ISBN No: 2582-9459

सीबीएमआर
CBMR

Advancing Frontiers of Science for Human Health and Wellness©

वार्षिक प्रतिवेदन
Annual Report
2022

जैव चिकित्सा अनुसंधान केन्द्र
Centre of BioMedical Research


विज्ञान और प्रौद्योगिक
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Published by
Director
Centre of BioMedical Research
SGPGIMS Campus, Raebareli Road, Lucknow – 226014, U.P. (INDIA)
Email: director.cbmr@cbmr.res.in
Web: www.cbmr.res.in

ISSN No: 2582-9459

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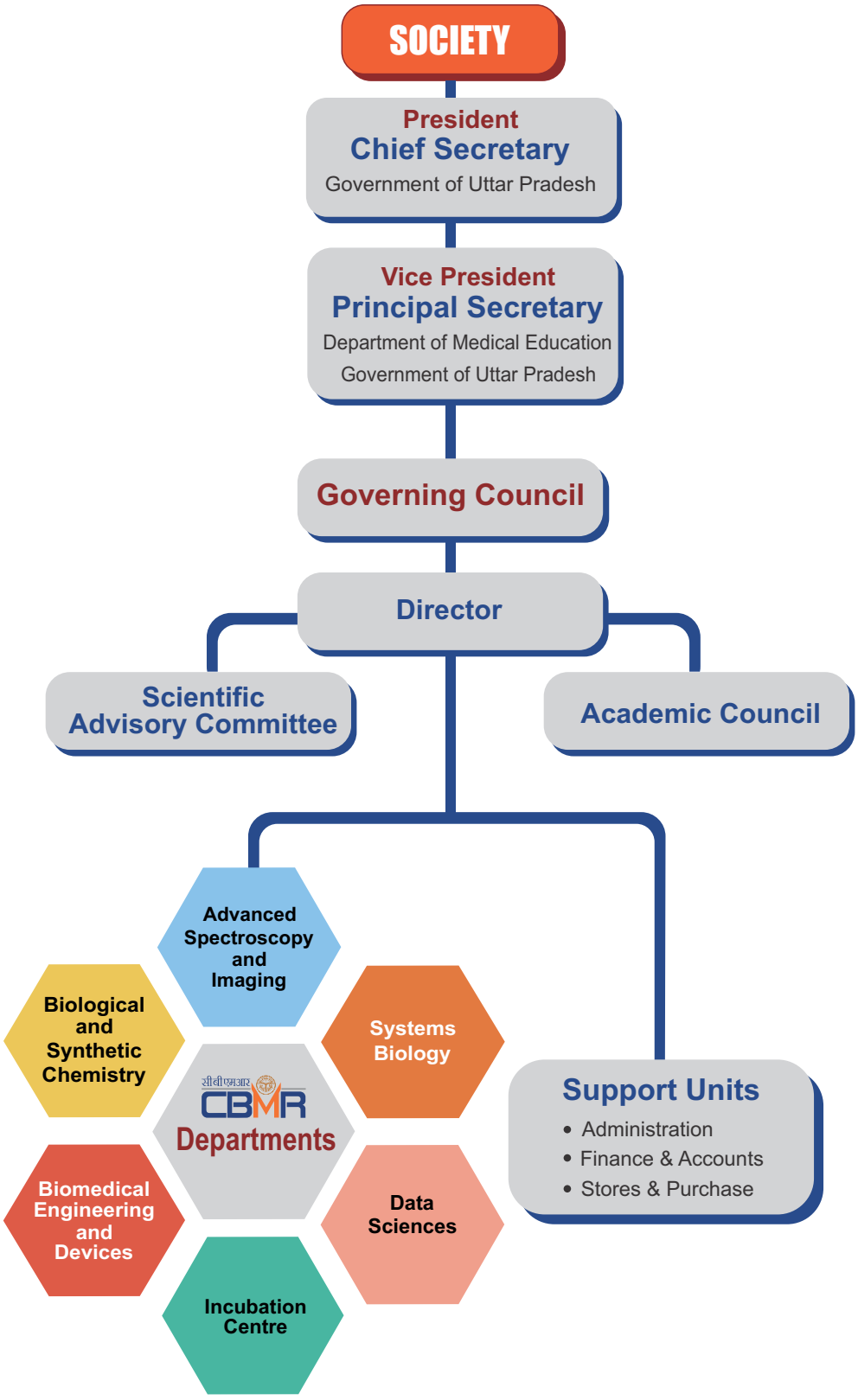
Organisational Structure



From the Director's Desk

It is a pleasure to present the Annual Report of CBMR which is "*Advancing Frontiers of Science for Human Health and Wellness.*"© During the year 2022, CBMR initiated new research areas and translational studies for better patient care.

The CBMR Governing Council approved the upgradation of CBMR to an institute on priority with the following six departments as per the scientific needs of the country, Department of Data Sciences, Department of Biomedical Engineering and Devices, Department of Advanced Spectroscopy and Imaging, Department of Biological & Synthetic Chemistry, Department of Systems Biology, and an Incubation Centre.

A 3D bioprinting facility was established at CBMR to enable the fabrication of complex three-dimensional (3D) structures for a variety of biomedical applications such as tissue engineering and therapeutic testing.

A high-performance computing (HPC) cluster funded by Department of Science and Technology (DST), Ministry of Science and Technology, Government of India, was established for the analysis of structural and functional imaging data, including cognitive functions of patients obtained from 3T-fMRI.

The Department of Science and Technology (DST), Ministry of Science and Technology, Government of India, has accepted the establishment of a DST-Satellite Center for Policy Research at CBMR. This will allow for developing a robust STI Policy for Uttar Pradesh in consultation with stake holders including the Government. Once the policy is released, it will provide a boost to the science and innovation ecosystem even in the rural areas of the State.

Some of the highlights of the scientific achievements in the reporting period include a series of powerful catalysts and ligands prepared to solve the challenging and long-standing problems associated with the C-H bond activation and functionalization chemistry, especially, C-H borylation chemistry *(Angewandte Chemie International Edition 2022, 61, e202203539; Organic Letters 2022, 24, 8147)*. These catalysts and ligands would certainly find a wide application in the context of drug diversification, medicinal chemistry as well as in the pharmaceutical industries. These catalysts/ligands have been protected by filing of patents. Development of multienzyme cascade strategy for the synthesis of complex natural products is an upcoming research area in biocatalysis. Recently, a highly efficient one-pot multienzyme cascade reaction is developed for the synthesis of natural naphthalenones *(ACS Catalysis 2022, 12(19), 12179)*. In addition, the first synthesis of some of the highly complex natural products such as luteoskyrin and deoxyluteoskyrin were synthesized using a chemoenzymatic strategy, which was inspired by the natural biosynthesis *(Tetrahedron Chem. 2022, 3, 100030)*. Moreover, a series of new concepts and methods were developed at the Centre to make high-value nitrogen-heterocycles that would find applications in drug discovery and medicinal chemistry *(Journal of the American Chemical Society 2022, 144, 21858; Chemical Science 2022, 13, 11817; Chemical Communications 2022, 58, 2504 & 7538; Advanced Synthesis & Catalysis 2022, 364, 41; 391, 3035 & 4031; Chemistry - A European Journal 2022, 28, e202201208)*.

A concise and scalable total synthesis of eupalinilde E in 12 steps with a high overall yield from commercially available (R)-(-)-carvone was developed to study the *ex vivo* and *in vivo* production of human hematopoietic stem and progenitor cells (HSPCs), which can improve the success of bone marrow transplants and the treatment of various blood diseases

and disorders *(Organic Letters 2022, 24, 8147).* Eupalinilide E is a sesquiterpene lactone that enhances the HSPCs expansion. A patent on this work has also been filed. This work was highlighted in ChemistryViews, The Magazine of Chemistry Europe, Willey-VCH (July 05, 2022).

Dose limiting cardiotoxicity remains a major limiting factor in the clinical use of cancer chemotherapeutics. Research at CBMR showed that G-protein regulator RGS11 protein forms complex with apoptotic kinase CaMKII and triggers mitochondrial dysfunction *(Redox Biology, 2022, 57, 102487).* Self-assembled structures composed of amphipathic, charged tripeptides were developed for intracellular delivery of pro-apoptotic chemotherapeutics (*Israel Journal of Chemistry, 2022, 62 (9-10), e202200001*). Further, due to the selective myocyte-intrinsic and myocyte-extrinsic actions, RGS7 in heart was found to be an attractive therapeutic target in the mitigation of chemotherapy-driven cardiotoxicity *(PNAS, 2022, 120 (1) e2213537120*).

A study was conducted using 3T-fMRI to understand the neuronal connectivity in children with ADHD and children with bipolar disorder. Abnormal connectivity patterns were observed in children with ADHD. This provided potential insights into the underlying neural mechanisms responsible for cognitive deficits and could lead to the development of personalized treatments *(Neuroimaging, 2022, 326, 111531)*. Similarly, research on children with bipolar disorder has demonstrated the benefits of using surface-based morphometric analysis on brain structural MRI data to identify morphological changes in the brain *(Asian Journal of Psychiatry, 2022, 80, 103352)*.

NMR based metabolomics approach was utilized to understand the metabolic profiles in the septic shock patients. Novel understanding in the progression of sepsis due to comorbidity conditions were obtained by the serum metabolic profiles of these patients which will help in the treatment of sepsis *(Mol. Omics, 2022, 18, 143)*. Clinical metabolomics was used to identify unique metabolic signatures of diagnostic potential in lung cancer *(ACS Omega 2022, 7(6), 5510)* and endometriosis *(ACS Omega 2022, 7(17), 14856)*. Metabolome of the cerebrospinal fluid from tuberculosis (TB) meningitis patients was found to be perturbed as unveiled by ^{1}H NMR-based metabolomics and the roles of various metabolites in the disease progression were deciphered *(Metabolic Brain Disease, 2022, 37(3), 773*). A new method to improve the quantitative ability of two-dimensional (2D) NMR was developed for resolving complex mixtures and was found to have a distinct advantage over one-dimensional (1D) ^{1}H NMR *(Journal of Magnetic Resonance Open*, *2022 12-13, 100063)*. Using a novel method of slice selection, the resolution of *J*-Resolved NMR spectra was enhanced *(Journal of Magnetic Resonance 2022, 342, 107267)*.

The academic activity of the Institute was well supported by a team of motivated and dedicated faculty members, who published 70 research articles in peer-reviewed national and international journals with an average impact factor of 5.73, along with two books, and book chapters. *One of the review articles on borylation chemistry was published in Chemical Society Reviews with an impact factor of >60*. Also, an original research article pertaining to "A RGS7-CaMKII complex drives myocyte-intrinsic and myocyte-extrinsic mechanisms of chemotherapy-induced cardiotoxicity" was accepted for publication in one of the most prestigious journals, *Proceedings of the National Academy of Sciences, USA (PNAS)*. Apart from this, two research articles were published in impact factor >15 and three in > 10 and eighteen in > 5. Further, the faculty members of the Centre have filed five patents, and two were granted during the year.

Six PhD students were awarded degrees and eleven project students received training. To augment the research and translational potential, the Centre has signed memorandum of understanding (MoU) with several institutions including IIT-Kanpur, IIT-Bombay, DBT-THSTI etc.

The faculty have supported their research through 20 ongoing extramural research projects worth > ₹975 lakhs. As part of CBMR's scientific societal responsibility, undergraduate and postgraduate students from various institutions visited the Centre to experience first-hand the research being undertaken.

A two-day national event on "Women Driving Science and Technology in India" was organized by CBMR under the aegis of the Science and Engineering Research Board (SERB), New Delhi on August 25-26, 2022. It was the first event of its kind in the state of Uttar Pradesh. Approximately 200 post-doctoral and early career women faculty attended the conference and became acquainted with the existing and potential S&T opportunities for women in both academic and corporate sectors in India.

A hands-on training workshop on "Recent Advances in 3D Bio-Printing of Living Tissues and its Emerging Applications in Biomedical Research" was organised. The workshop was attended by PhD students, academic research scholars, and faculty members from various institutions.

"Vigyan Sangam", a lecture series was initiated to celebrate *Azadi Ka Amrit Mahotsav*. Renowned scientists gave lectures at CBMR for the benefit of faculty and students towards developing further research collaboration in niche areas of science and technology.

CBMR celebrated 75 years of India's Independence under the theme *"Azadi Ka Amrit Mahotsav"* by organizing a series of events from August 11–17, 2022. Several activities were undertaken on the National Science Day, National Technology Day, and International Day of Yoga etc. with active participation of the faculty, staff and students of CBMR. The Road Safety Week was also observed at CBMR, in alignment with the mandate of the Ministry of Road Transport & Highways and Government of Uttar Pradesh, from April 18-24, 2022.

CBMR has successfully established itself as the leading research and development organization in the country, playing a key role in responding to societal needs and better patient care. Through the efforts of the CBMR faculty and staff, we would like to ensure that the Center remains globally positioned in the niche areas of biology and chemistry. I am confident that CBMR will continue to grow in line with its vision and mission to meet the needs of State and National mission programmes.

I am indeed grateful to the President CBMR and Chief Secretary, Uttar Pradesh for constantly guiding CBMR as the Chairperson of the Governing Council. I should like to place on record my deep sense of gratitude to the Principal Secretary, Department of Medical Education, Government of Uttar Pradesh and Director General, Medical Education for providing constant guidance and support to CBMR. I also extend my heartfelt gratitude to the Chairman and Members of the CBMR Governing Council as well as Scientific Advisory Committee (SAC) for their guidance and suggestions to the Centre. I am extremely grateful to the Hon'ble Chief Minister, Government of Uttar Pradesh; Hon'ble Cabinet Minister and Hon'ble State Minister, Department of Medical Education for their continued guidance and unstinted support to CBMR.

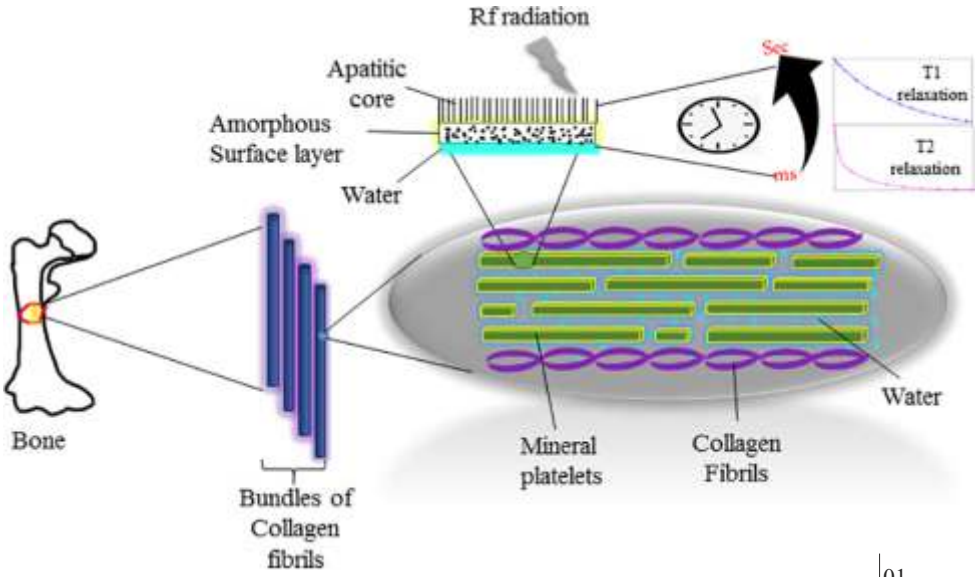
(Alok Dhawan)

Research Highlights

Unraveling Water-Mediated ^{31}P Relaxation in Bone Mineral

Navneet Dwivedi, Richa Dubey, Seema Srivastava, Neeraj Sinha (2022).
ACS Omega, 7 (19): 16678 – 16688

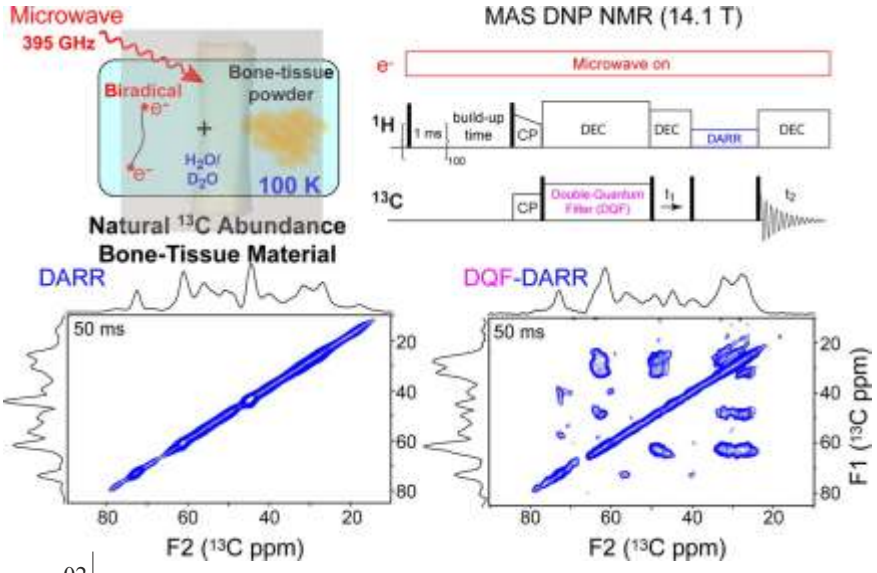
Bone is a dynamic tissue composed of organic proteins (mainly type I collagen), inorganic components (hydroxyapatite), lipids, and water that undergoes a continuous rebuilding process over the lifespan of human beings. Bone mineral is mainly composed of a crystalline apatitic core surrounded by an amorphous surface layer. The supramolecular arrangement of different constituents gives rise to its unique mechanical properties, which become altered in various bone-related disease conditions. Many of the interactions among the different components are poorly understood. Recently, solid-state nuclear magnetic resonance (ssNMR) has become a popular spectroscopic tool for studying bone. In this article, we present a study probing the interaction of water molecules with amorphous and crystalline parts of the bone mineral through ^{31}P ssNMR relaxation parameters (T_1 and T_2) and dynamics (correlation time). The method was developed to selectively measure the ^{31}P NMR relaxation parameters and dynamics of the crystalline apatitic core and the amorphous surface layer of the bone mineral. The measured ^{31}P correlation times (in the range of 10^6–10^7 s) indicated the different dynamic behaviors of both the mineral components. Additionally, we observed that dehydration affected the apatitic core region more significantly, while H–D exchange showed changes in the amorphous surface layer to a greater extent. Overall, the present work provides a significant understanding of the relaxation and dynamics of bone mineral components inside the bone matrix.



Dynamic nuclear polarization-enhanced, double-quantum filtered ^{13}C-^{13}C dipolar correlation spectroscopy of natural ^{13}C abundant bone issue biomaterial

Sungsool Wi, Navneet Dwivedi, Richa Dubey, Frederic Mentink-Vigier, Neeraj Sinha (2022). ***Journal of Magnetic Resonance***, 335:107144.

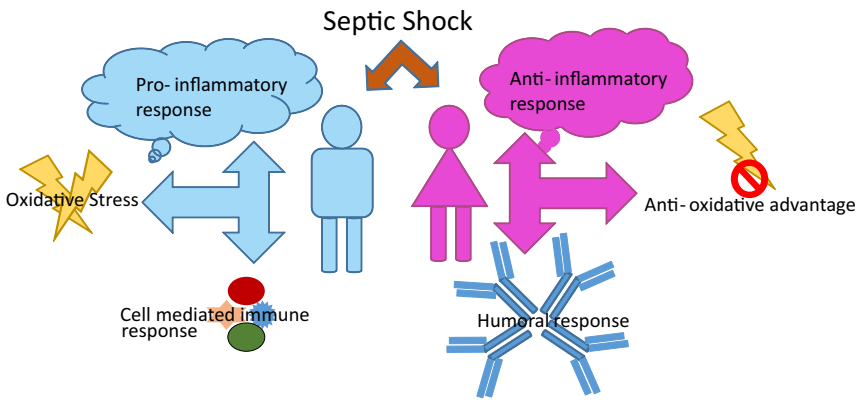
Here, we describe a method for obtaining a dynamic nuclear polarization (DNP)-enhanced doublequantum filtered (DQF) two-dimensional (2-D) dipolar ^{13}C-^{13}C correlation spectra of bone-tissue material at natural ^{13}C abundance. DNP-enhanced DQF 2D dipolar ^{13}C-^{13}C spectra were obtained using a few different mixing times of the dipolar-assisted rotational resonance (DARR) scheme and these spectra were compared to a conventional 2-D through-space double-quantum (DQ)-single-quantum (SQ) correlation spectrum. While this scheme can only be used for an assignment purpose to reveal the carbon-carbon connectivity within a residue, the DQF ^{13}C-^{13}C dipolar correlation scheme introduced here can be used to obtain longer distance carbon-carbon constraints. A DQF pulse block is placed before the DARR mixing scheme for removing dominant ^{13}C single-quantum (SQ) signals because these SQ ^{13}C signals are overwhelmingly large compared to those ^{13}C-^{13}C dipolar cross-peaks generated and therefore saturate the dynamic range of the NMR detection. This approach exhibits strong enough 2-D cross-peaks in a dipolar ^{13}C-^{13}C correlation spectrum and potentially provides pairwise ^{13}C-^{13}C dipolar constraints because the dipolar truncation effect as well as multi-step signal propagations involving a spin cluster that contains more than two spins can be ignored probabilistically. To obtain fast signal averaging, Asym Pol POK was used to provide a short ^{1}H DNP signal build-up time (1.3 s) and to expedite our MAS DNP NMR acquisitions while still maintaining a satisfactory DNP enhancement factor (e = 50). Under long DARR mixing, a t_1-noise-like artifact was observed at a site that possesses a large chemical shift anisotropy (CSA) and a few different strategies to address this problem were discussed.



Gender-specific association of oxidative stress and immune response in septic shock mortality using NMR-based metabolomics

Swarnima Pandey, Mohd Adnan Siddiqui, Surendra Kumar Trigun, Afzal Azim, Neeraj Sinha (2022).
Molecular Omics, 18 (2): 143-153.

Sepsis and septic shock are still associated with a high mortality rate. The early-stage prediction of septic shock outcomes would be helpful to clinicians for designing their treatment protocol. In addition, it would aid clinicians in patient management by understanding gender disparity in terms of clinical outcomes of septic shock by identifying whether there are sex-based differences in sepsis-associated mortality. *Objective*: This study aimed to test the hypothesis that gender-based metabolic heterogeneity is associated with sepsis survival and identify the biomarkers of mortality for septic shock in an Indian cohort. *Method*: The study was performed in an Indian population cohort diagnosed with sepsis/septic shock within 24 hours of admission. The study group was 50 patients admitted to intensive care, comprising 23 females and 27 males. Univariate and multivariate analysis were performed to identify the biomarkers for septic shock mortality and the gender-specific metabolic fingerprint in septic shock-associated mortality. *Results*: The energy-related metabolites, ketone bodies, choline, and NAG were found to be primarily responsible for differentiating survivors and non-survivors. The gender-based mortality stratification identified a female-specific association of the anti-inflammatory response, innate immune response, and β oxidation, and a male-specific association of the pro-inflammatory response to septic shock. *Conclusion*: The identified mortality biomarkers may help clinicians estimate the severity of a case, as well as predict the outcome and treatment efficacy.



The study underlines that gender is one of the most significant biological factors influencing septic shock metabolomics profiles. This understanding can be utilized to identify novel gender-specific biomarkers and innovative targets relevant for gender medicine.

Metabolic fingerprint of patients showing responsiveness to treatment of septic shock in intensive care unit

Swarnima Pandey, Mohd Adnan Siddiqui, Afzal Azim, Neeraj Sinha (2022). ***Magnetic Resonance Materials in Physics Biology and Medicine***, 1-11.

An early metabolic signature associated with the responsiveness to treatment can be useful in the better management of septic shock patients. This would help clinicians in designing personalized treatment protocols for patients showing non-responsiveness to treatment.

Methods

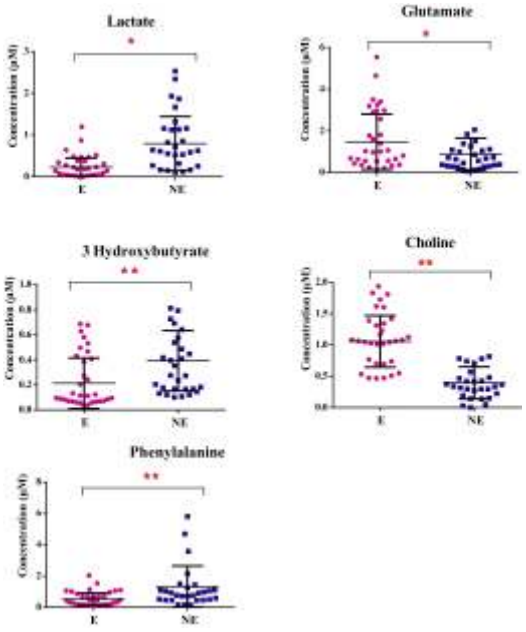
We analyzed the serum on Day 1 ($n = 60$), Day 3 ($n = 47$), and Day 5 ($n = 26$) of patients with septic shock under treatment using NMR-based metabolomics. Partial least square discriminant analysis (PLS-DA) was performed to generate the list of metabolites that can be identified as potential disease biomarkers having statistical significance (that is, metabolites that had a VIP score > 1, and p value < 0.05, False discovery rate (FDR) < 0.05).

Results

Common significant metabolites amongst the three time points were obtained that distinguished the patients being responsive (R) and non-responsive (NR) to treatments, namely 3 hydroxybutyrate, lactate, and phenylalanine which were lower, whereas glutamate and choline higher in patients showing responsiveness.

Discussion

The study gave these metabolic signatures identifying patients' responsiveness to treatment. The results of the study will aid in the development of targeted therapy for ICU patients.



Nuclear magnetic resonance spectroscopy reveals dysregulation of monounsaturated fatty acid metabolism upon SPINK1 attenuation in colorectal cancer

Shivansh Nigam, Renuka Ranjan, Neeraj Sinha, Bushra Ateeq (2022). ***NMR in Biomedicine***, 35 (7): e4705.

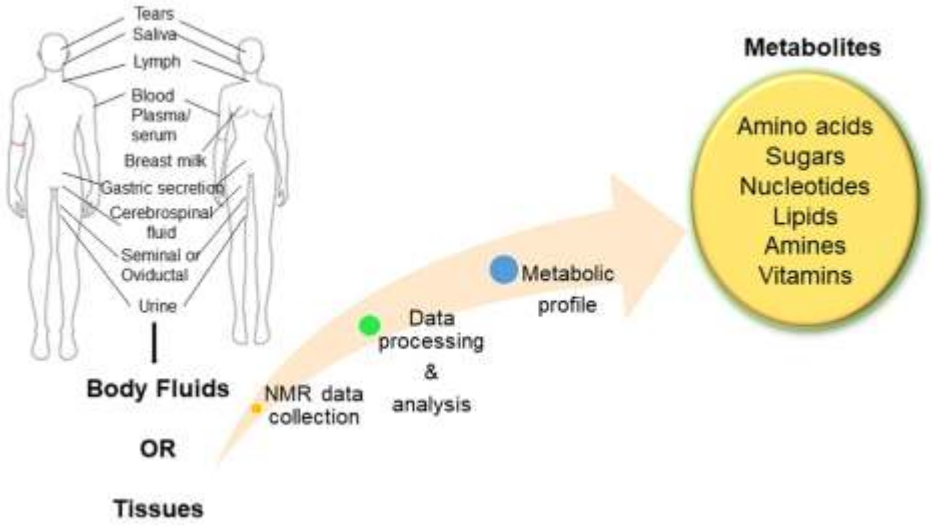
Metabolic reprogramming, a key hallmark of cancer, plays a pivotal role in fulfilling the accelerated biological demands of tumor cells. Such metabolic changes trigger the production of several proinflammatory factors, thereby inciting cancer development and its progression. Serine protease inhibitor Kazal Type 1 (SPINK1), well known for its oncogenic role and its upregulation via acute-phase reactions, is highly expressed in multiple cancers including colorectal cancer (CRC). Here, we show accumulation of lipid droplets in CRC cells stained with Oil Red O upon SPINK1 silencing. Furthermore, NMR spectroscopy analysis revealed an accretion of monounsaturated fatty acids (MUFAs) and phosphatidylcholine in these CRC cells, while the levels of polyunsaturated fatty acids remained unaltered. This alteration indicates the presence of MUFAs with the triglycerides in the lipid droplets as observed in SPINK1-silenced CRC cells. Considering the role of MUFAs in the anti-inflammatory response, our data hint that suppression of SPINK1 in CRC leads to activation of an anti-inflammatory signaling milieu. Conclusively, our study uncovers a connection between lipid metabolism and SPINK1-mediated CRC progression, hence paving the way for further exploration and better prognosis of SPINK1-positive CRC patients.

Potential of *in vitro* NMR of bio fluids and tissues in clinical research

Richa Dubey, Neeraj Sinha, Naranamangalam R. Jagannathan
(2022). ***NMR in Biomedicine***, 36 (4):e4686

Body fluids, cells, and tissues contain a wide variety of metabolites that consist of amixture of various low-molecular-weight compounds, including amino acids, peptides, lipids, nucleic acids, and organic acids, which makes comprehensive analysis more difficult. Quantitative nuclear magnetic resonance (NMR) spectroscopy is a well-established analytical technique for analyzing the metabolic profiles of body fluids, cells, and tissues. It enables fast and comprehensive detection, characterization, a high level of experimental reproducibility, minimal sample preparation, and quantification of various endogenous metabolites. In recent times, NMR-based metabolomics has been appreciably utilized in diverse branches of medicine, including microbiology, toxicology, pathophysiology, pharmacology, nutritional intervention, and disease diagnosis/prognosis. In this review, the utility of NMR-based metabolomics in clinical studies is discussed. The significance of in vitro NMR-based metabolomics as an effective tool for detecting metabolites and their variations in different diseases are discussed, together with the possibility of identifying specific biomarkers that can contribute to early detection and diagnosis of disease.

Figure 1



High mobility group box 1 (HMGB1) inhibition attenuates lipopolysaccharide-induced cognitive dysfunction and sickness-like behavior in mice

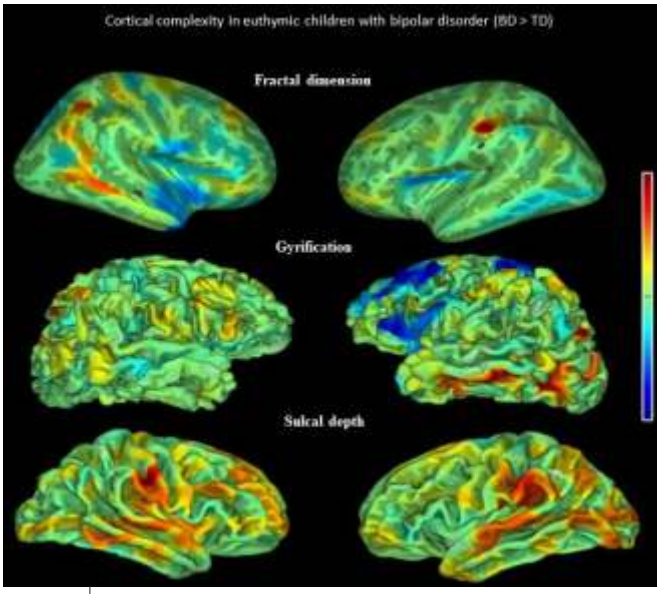
Devlina Ghosh, Aditi Singh, Alok Kumar, Neeraj Sinha (2022). ***Immunologic Research***, 70: 633–643.

Cognitive dysfunction, sickness-like behavior, for instance, anxiety, and depression are common aspects of neuropsychiatry often associated with neurodegenerative disorders. Growing evidence suggests that high mobility group box 1 (HMGB1) may act as a proinflammatory cytokine that aggravates neurobehavioral dysfunction. However, the detailed underlying mechanism is still elusive. Here we focus on determining the relationship between lipopolysaccharide (LPS)-induced neuroinflammation (in both in vitro and in vivo models), cognitive dysfunction, sickness-like behavior and thus decode the impact of HMGB1 inhibition (using Glycyrrhizin; Gcy as an antagonist). Using a mice model of repeated LPS (1 mg/kg, i.p. for 4 days) injections, we found that LPS induced neurobehavioral deficit and a strong proinflammatory response with increased proinflammatory markers, including tumor necrosis factor-α (TNF-α), interleukin-1 beta (IL-1β), interleukin-6 (IL-6) and iNOS (inducible nitric oxide synthase) at 7 days after the final dose of LPS compared to control animals. Our findings suggest that neurobehavioral dysfunction strongly correlates with the proinflammatory immune response following LPS stimulation. In vitro Gcypretreatment to LPS-activated BV2 microglia cells significantly reduced nitrite and reactive oxygen species production, along with diminished expression of classical proinflammatory cytokines (TNF-α, IL-1β, IL-6, iNOS). These key proinflammatory changes with LPS and Gcy treatment are also found in vivo mice model and correlate with improved cognitive function and reduced anxiety/depression. Together, these results show that blocking HMGB1 using Gcy abrogated the cognitive dysfunction, sickness-like behavior of anxiety and depression induced by LPS which can be a promising avenue for crucial neurobehavioral dysfunction.

Computing brain cortical complexity in euthymic children with bipolar disorder: A surface-based approach.

Anshita Singh, Amit Arya, Vivek Agarwal, Raj Shree, Uttam Kumar (2022). ***Asian Journal of Psychiatry,*** 80: 103352

Bipolar disorder (BD) beginning in childhood or early adolescence is a rarer and more severe form of psychiatric disorder than adult-onset BD. The former is characterized by episodes of elevated/irritable mood and those of depression, which exceed what is expected for the child's development. There may be symptoms of mood dysregulation, state of continuous irritability, and rapid cycling. In the manic phase, patients with BD are very active, happy, irascible, and hardly need sleep. On the other side of this disorder is depression, in which the patient experiences drowsiness and develops an inferiority complex (Grande et al., 2016). Pediatric bipolar disorder may lead to considerable disruption of normal development and psychosocial functioning. The patient may improve with adequate treatment and remain in a relatively normal stage known as the euthymic phase. However, in this phase, the clinical symptoms are not entirely absent and are merely diminished to the extent that mood and daily behavior are not affected. Cognitive impairment in various aspects, such as executive functioning, verbal and visual memory, and maintaining focus, psychomotor speed, and visuospatial abilities may be compromised during the euthymic phase (Bhatia et al., 2018). Structural brain analysis in children with euthymic BD revealed alterations in frontal, temporal, parietal, and occipital regions in terms of increase or decrease in gray and white matter volume and cortical thickness (Singh et al., 2022; Achalia et al., 2020). Imaging studies on the brain grey and white matter using voxel-based morphometric analysis are available in BD but are limited in children and adolescents. In such cases, additional surface-based cortical analysis apart from volumetric measures may provide crucial information on children with BD. Thus, we performed three interrelated morphometric analyses to measure sulcus depth, gyrification index, and fractal dimension and quantify the cortical abnormalities. These three analyses were expected to provide information on shape and complexity changes in the brain, degree of regional folding in the human brain, any shrinkage in the gyri, and certain distal changes that might affect the brain's global shape.

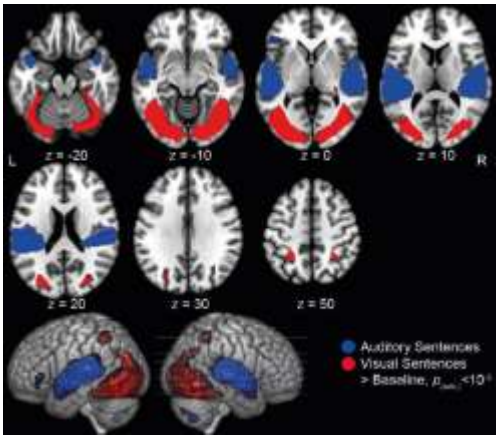


How does literacy affect speech processing? Not by enhancing cortical responses to speech, but by promoting connectivity of acoustic-phonetic and graphomotor cortices.

Alexis Hervais-Adelman, Uttam Kumar, Ramesh K Mishra, Viveka N Tripathi, Anupam Guleria, Jay P Singh, Falk Huettig (2022). ***Journal of Neuroscience***, 42 (47): 8826-8841.

Previous research suggests that literacy, specifically learning alphabetic letter-to-phoneme mappings, modifies online speech processing and enhances brain responses, as indexed by the BOLD, to speech in auditory areas associated with phonological processing (Dehaene et al., 2010). However, alphabets are not the only orthographic systems in use in the world, and hundreds of millions of individuals speak languages that are not written using alphabets. In order to make claims that literacy per se has broad and general consequences for brain responses to speech, one must seek confirmatory evidence from non-alphabetic literacy. To this end, we conducted a longitudinal fMRI study in India probing the effect of literacy in Devanagari, an abubgida, on functional connectivity and cerebral responses to speech in 91 variously literate Hindi-speaking male and female human participants. Twenty-two completely illiterate participants underwent 6 months of reading and writing training. Devanagari literacy increases functional connectivity between acoustic-phonetic and graphomotor brain areas, but we find no evidence that literacy changes brain responses to speech, either in cross-sectional or longitudinal analyses. These findings show that a dramatic reconfiguration of the neurofunctional substrates of online speech processing may not be a universal result of learning to read, and suggest that the influence of writing on speech processing should also be investigated.

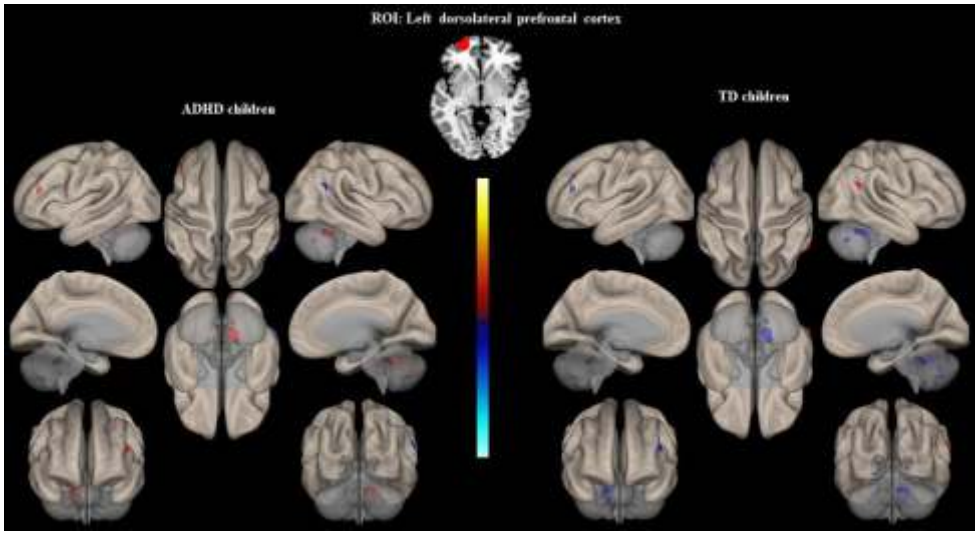
SIGNIFICANCE STATEMENT: It is widely claimed that a consequence of being able to read is enhanced auditory processing of speech, reflected by increased cortical responses in areas associated with phonological processing. Here we find no relationship between literacy and the magnitude of brain response to speech stimuli in individuals who speak Hindi, which is written using a non-alphabetic script, Devanagari, an abugida. We propose that the exact nature of the script under examination must be considered before making sweeping claims about the consequences of literacy for the brain. Further, we find evidence that literacy enhances functional connectivity between auditory processing areas and graphomotor areas, suggesting a mechanism whereby learning to write might influence speech perception.



Altered functional connectivity in children with ADHD while performing cognitive control task

Uttam Kumar, Amit Arya, Vivek Agarwal (2022). ***Neuroimaging***, 326:111531

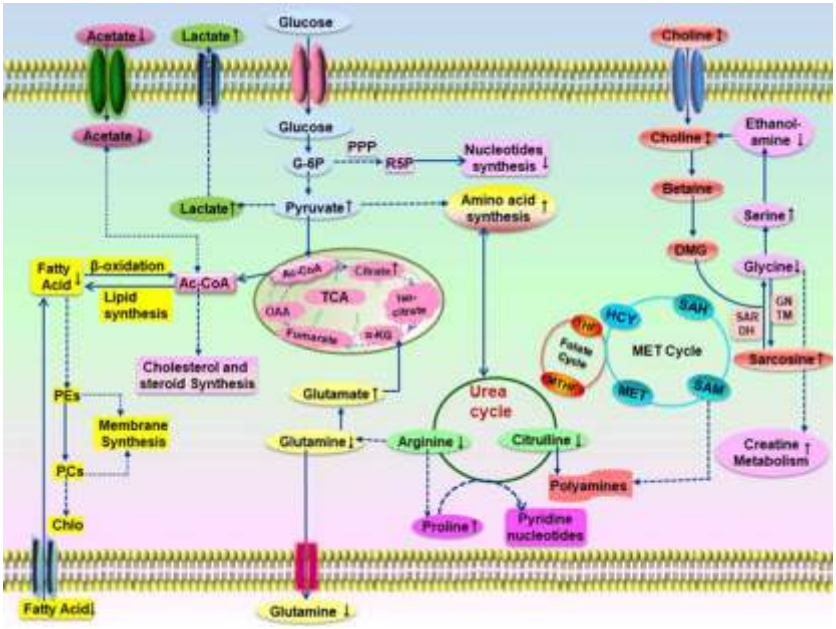
Response inhibition is one of the crucial cognitive domains that exhibit deficit in children with ADHD. To further elucidate it, this study examines the task-based functional-connectivity in children with attention deficit hyperactive disorder (ADHD). We acquired the fMRI data of 16 un-medicated children with ADHD and 16 typically developing (TD) children who performed the flanker task. MVPA and seed-based connectivity analysis was performed to identify the abnormal connectivity pattern across the whole brain. MVPA revealed that six important regions, namely the right IFG, right SMA, bilateral precentral gyrus, left DLPFC, and left cerebellum, had abnormal connectivity in children with ADHD while they performed the cognitive control task. Out of these six regions, four were further used for whole-brain seed-based functional connectivity analyses, which revealed patterns of significantly altered connectivity across multiple regions. Signal intensities changes were also extracted to perform BOLD- reaction time (RT) correlation analysis, that suggest positive correlation between left DLPFC and right IFG. Overall, the results suggest that children with ADHD are unable to endure high cognitive control demand. Our findings highlight the utility of analyzing brain connectivity data in identifying the abnormal connectivity in children with ADHD.



Relevance of Emerging Metabolomics-Based Biomarkers of Prostate Cancer: A Systematic Review

Navneeta Bansal, Manoj Kumar, S N Sankhwar, Ashish Gupta (2022). ***Expert Reviews in Molecular Medicine***, 24: e25.

Prostate cancer (PC) presents great challenges in early diagnosis and often leads to unnecessary invasive procedures as well as over diagnosis and treatment, thus highlighting the need for promising early diagnostic biomarkers. The aim of this review is to provide an up-to-date summary of chronologically existing metabolomics PC biomarkers, their potential to improve clinical PC diagnosis, and to reduce the proliferation and monitoring of PC. The systematic research was conducted on PubMed in accordance with PRISMA guidelines to report PC biomarkers. The majority of the studies distinguished malignant from benign prostate and few explored the biomarkers associated with the progression of PC. The present review summarizes the primary outcomes of most significant studies to extend our knowledge of PC metabolomics biomarkers. We observed divergent inter-laboratory technical procedures employing different statistical approaches produced abundant information regarding PC metabolites perturbation. Since PC metabolomics is still in its early phase, it is vital that we dig out the most specific, sensitive, and accurate metabolic signatures and conduct more studies with milestone findings with comparable sample sizes to validate and corroborate the findings.

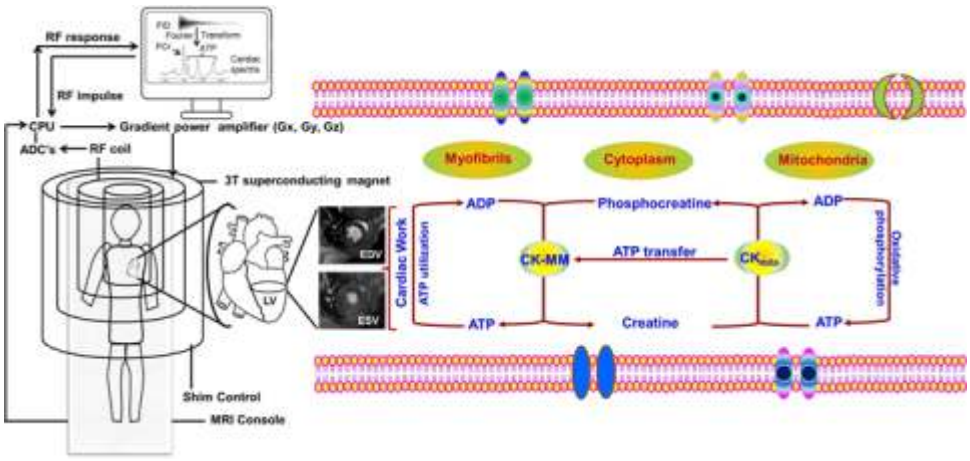


A typical contributory metabolic pathways and their intermediate metabolites involved in metabolism of PC. Up-regulated and down-regulated metabolites are depicted with (↑) and (↓), respectively.

Cardiac ^{31}P MR Spectroscopy: Development of the Past Five Decades and Future Vision Will it be of Diagnostic Use in clinics

Ashish Gupta (2022).
Heart Failure Reviews, 28: 485–532

In the past five decades, the use of the magnetic resonance (MR) technique for cardiovascular diseases has engendered much attention and raised the opportunity that the technique could be useful for clinical applications. MR has two arrows in its quiver: one is magnetic resonance imaging (MRI) and other is magnetic resonance spectroscopy (MRS). Highly advanced MRI provides unique and profound information about the anatomical changes of the heart non-invasively. Excellently developed MRS offers irreplaceable and insightful evidence of real-time biochemistry of cardiac metabolism of underpinning diseases. Compared to MRI, which has already been successfully applied in routine clinical practice, MRS still has a far distance to travel to be incorporated into routine diagnostics. Considering the exceptional potential of 31P MRS to measure the real-time metabolic changes of energetic molecules qualitatively and quantitatively, how far its powerful technique should be waited before successful transition from "bench-to-bedside" is enticing. The present review highlights the seminal studies on the chronological development of cardiac 31P MRS in the past five decades and the future vision and challenges to incorporate it for routine diagnostics of cardiovascular disease.



Schematic approach for the cardiac 31P MRS using as a probative technique. CK-MM creatine kinase isoenzyme, CKmito creatine kinase mitochondrial isoenzyme, ATP adenosine triphosphate, ADP adenosine diphosphate, LV left ventricle, EDV end diastolic volume, ESV end systolic volume

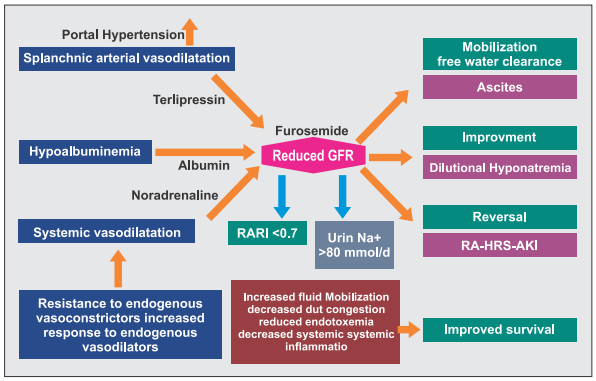
Response guided slow infusion of albumin, asoconstrictors and furosemide improves ascites mobilization and survival in acute on chronic liver failure: a proof-of-concept study

Gaurav Pande, Manjunath Hatti, Mohit Kumar Rai, Praveer Rai, Kamlesh Kumar, V.P Krishna, Abhimanyu Nehra, Sudeep Kumar, Sourav Kumar Mishra, Dinesh Kumar, Umesh Kumar, Prabhakar Mishra, Abdul Majeed, Vivek Anand Saraswat, Kritika Singh, Harshit Singh, Durga Prasanna Misra and Vikas Agarwal (2022). ***Journal of Inflammation Research***, 15: 5027–5039

Background and Aims: Acute-on-chronic liver failure (ACLF) with increasing organ failure is associated with poor outcomes. Severely deranged systemic hemodynamics and decreased effective arterial blood volume contribute to tissue damage and organ failure. Response-guided therapy with albumin, vasoconstrictors, and furosemide may help overcome effective hypovolemia, improve diuresis and impact survival. **Methods:** In the observation cohort, 230 patients with ACLF (CANONIC criteria) with ascites (≥Grade II) and ACLF ≥ Grade I were enrolled. A total of 136 patients (GROUP I) received response-guided (urine sodium > 80mmol/day) slow albumin-furosemide infusion ± terlipressin (SAFI ± T), while 94 patients (GROUP II) received standard medical therapy. Twenty-eight-day survival, ascites mobilization (nil or grade 1), and adverse events were noted. In another mechanistic cohort (n = 40), laboratory evidences for improvement in various pathophysiological alterations; gut permeability, endotoxemia, cytokine storm, neutrophil dysfunction, and hemodynamic alterations following SAFI ± T/Noradrenaline (NAdr) were evaluated.

Results: Age, gender, CLIF-C-ACLF, SOFA and MELD scores, ACLF grades and urine sodium were not different between the two groups in the observation cohort. Ascites was mobilized in 102/136 in GROUP I (SAFI ± T) and 23/94 in GROUP II ($p < 0.05$). Twenty-eight-day survival was significantly higher in GROUP I = 103/136 (75.7%) vs GROUP II = 50/94 (53.2%), (P = < 0.001). All those who were unable to reach urine sodium > 80 mmol/day died. Four patients in GROUP I developed scrotal gangrene. In the mechanistic cohort, 72% of patients survived with significant improvement in gut permeability, endotoxemia, serum cytokines, neutrophil dysfunction, and hemodynamic alterations.

Conclusion: Ascitic fluid mobilization by response-guided SAFI ± T/NAdr therapy improves survival by improving splanchnic and systemic hemodynamics, decreasing gut congestion, gut permeability, and endotoxemia, improving neutrophil functions, and reducing pro-inflammatory cytokines in circulation.

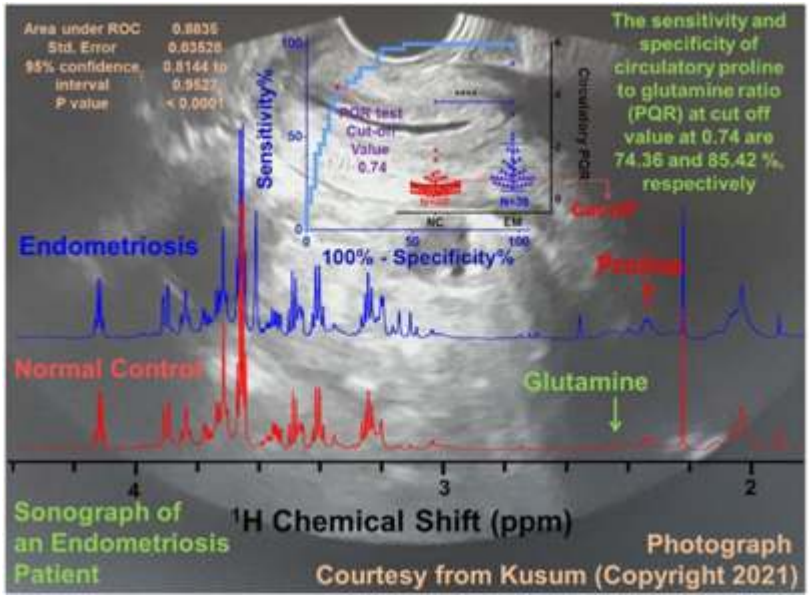


Underlying pathobiology of ascites in ACLF and its amelioration after proposed treatment.

Elevated Circulatory Proline to Glutamine Ratio (PQR) in Endometriosis and Its Potential as a Diagnostic Biomarker

Kusum Kusum, Ritu Raj, Sangeeta Rai, Pranjali Pranjali, Ashish Ashish, Sara Vicente-Muñoz, Radha Chaube and Dinesh Kumar (2022). ***ACS Omega***, 7 (17): 14856 –14866

Endometriosis (EM) is a hormone-dependent gynecological disease associated with chronic pelvic pain and altered immuno-inflammatory processes. It shares some cancer-like characteristics such as increased proline biosynthesis and activated glutaminolysis. Both proline and glutamine are interconvertible metabolically, and studies have shown their roles in cancer cell metabolic reprogramming, redox homeostasis, occurrence/development of endometrial carcinoma, and its further progression toward the malignant state. So based on this, we hypothesized that the circulatory proline to glutamine ratio (PQR) would be altered in EM and may serve as an indicative biomarker to improve the clinical diagnosis of EM. In present study, the circulatory-PQR levels were estimated for 39 EM patients and 48 age matched healthy female subjects using 800 MHz NMR spectroscopy. Among 39 EM patients, 15 were in the clinical stages I to II and referred to here as moderate EM (MEM) patients and 24 were in the clinical stages III to IV and referred here as severe EM (SEM) patients. The circulatory-PQR levels were significantly increased in EM patients (0.99 ± 0.13 μM in MEM; 1.39 ± 0.22 μM in SEM) compared to normal control (NC) subjects (0.52 ± 0.05 μM in NC). Further, the circulatory PQR levels exhibit the highest diagnostic potential with area under receiver operating characteristic (AUROC) curve values equal to 0.87 ± 0.04 [95%CI = 0.79–0.96] for MEM and 0.89 ± 0.04 [95% CI = 0.82–0.96] for SEM. These results suggested that circulatory-PQR has significant potential to serve as a noninvasive biomarker for diagnostic/prognostic screening of EM and further underscored the importance of these two nonessential amino acids (proline and glutamine) in cancer metabolism.

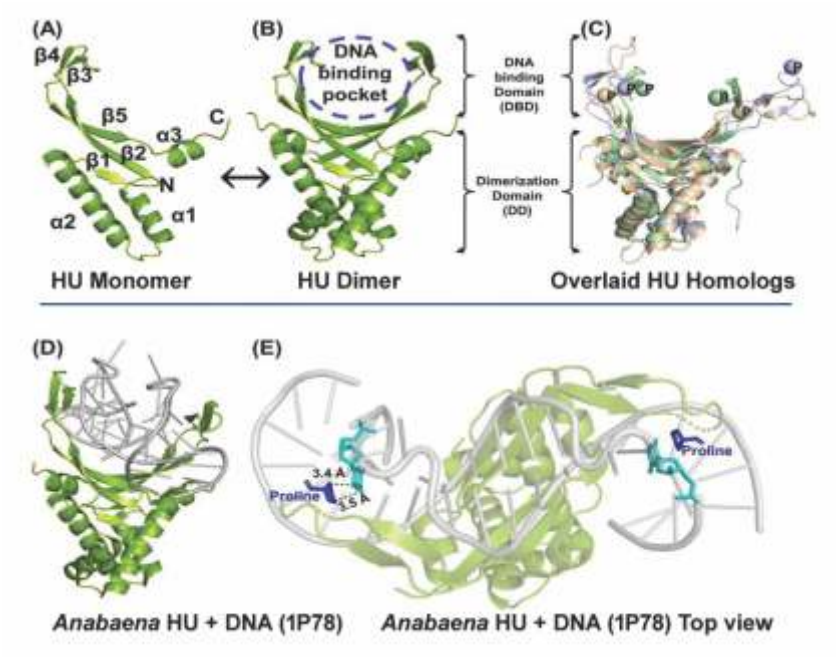


Diagnostic potential of circulatory Proline to Glutamine Ratio (PQR) evaluated for Endometriosis

Conserved apical proline regulates the structure and DNA binding properties of *Helicobacter pylori* Histone-like DNA binding protein (Hup)

Nipanshu Agarwal, Nupur Nagar, Ritu Raj, Dinesh Kumar, and Poluri, Krishna Mohan (2022). ***ACS Omega***, 7(17): 15231 –15246.

Prokaryotic cells lack a proper dedicated nuclear arrangement machinery. A set of proteins known as nucleoid associated proteins (NAPs) perform opening and closure of nucleic acids, behest cellular requirement. Among these, a special class of proteins analogous to eukaryotic histones popularly known as histone-like (HU) DNA binding proteins facilitate the nucleic acid folding/compaction thereby regulating gene architecture and gene regulation. DNA compaction and DNA protection in *Helicobacter pylori* is performed by HU protein (Hup). To dissect and galvanize the role of proline residue in the binding of Hup with DNA, the structure-dynamics-functional relationship of Hup-P64A variant was analyzed. NMR and biophysical studies evidenced that Hup-P64A protein attenuated DNA-binding and induced structural/stability changes in the DNA binding domain (DBD). Moreover, molecular dynamics simulations and 15N relaxation studies established the reduced conformational dynamics of P64A protein. This comprehensive study dissected the exclusive role of evolutionarily conserved apical proline residue in regulating the structure and DNA binding of Hup protein as P64 is presumed to be involved in the external leverage mechanism responsible for DNA bending and packaging, as proline rings wedge into the DNA backbone through intercalation besides their significant role in DNA binding.



Structural features of HU family proteins including Mycobacterium tuberculosis (green), Mycoplasma gallisepticum (peach), and Geobacillusstearo the rmophilus (purple) with their conserved

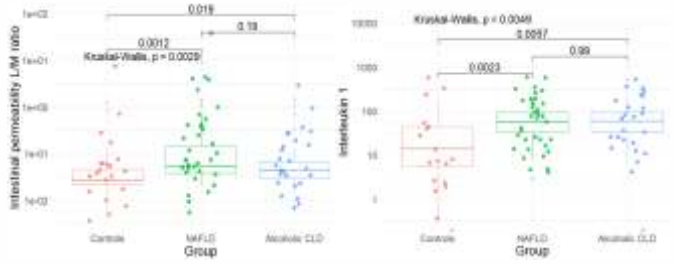
Demonstration of gut-barrier dysfunction in early stages of non-alcoholic fatty liver disease: A proof-of-concept study

Kanav Kaushal, Samagra Agarwal, Sanchit Sharma, Pooja Goswami, Namrata Singh, Vikas Sachdev, Shekhar Poudel, Prasenjit Das, Rajni Yadav, Dinesh Kumar, Gaurav Pandey, Deepak Gunjan, Anoop Saraya (2022). ***Journal of Clinical and Experimental Hepatology***, 12 (4):1102 – 1113

Background/Aims: Gut-barrier dysfunction is well recognized in pathogenesis of both non-alcoholic fatty liver disease (NAFLD) and alcoholic liver disease (ALD). However, comparison of components of this dysfunction between the two etiologies remains unexplored especially in early stages of NAFLD.

Methods: Components of gut-barrier dysfunction like alterations in intestinal permeability (IP) by lactulose mannitol ratio (LMR) in urine, systemic endotoxemia (IgG and IgM anti-endotoxin antibodies), systemic inflammation (serum tumor necrosis factor alpha [TNF-α] and interleukin-1 [IL-1] levels), tight junction (TJ) proteins expression in duodenal biopsy and stool microbiota composition using Oxford Nanopore MinION device were prospectively evaluated in patients with NAFLD (n = 34) with no cirrhosis, ALD (n = 28) and were compared with disease free controls (n = 20). **Results:**Patients with ALD had more advanced disease than those with NAFLD (median liver stiffness -NAFLD:7.1kPa [5.9–8.9] vs. ALD:14.3 kPa [9.6–24], P < 0.001]. Median LMR was significantly higher in NAFLD and ALD group when compared to controls (NAFLD 0.054 [0.037–0.17] vs. controls 0.027 [0.021–0.045] (P = 0.001)) and ALD 0.043 [0.03–0.068] vs. controls 0.027 [0.021–0.045] (P = 0.019)]. Anti-endotoxin antibody titer (IgM) (MMU/mL) was lowest in NAFLD 72.9 [3.2–1089.5] compared to ALD 120.6 [20.1–728]) (P = 0.042) and controls 155.3 [23.8–442.9]) (P = 0.021). Median TNF-α (pg/mL) levels were elevated in patients with NAFLD (53.3 [24.5–115]) compared to controls (16.1 [10.8–33.3]) (P < 0.001) and ALD (12.3 [10.1–42.7]) (P < 0.001). Expression of zonulin-1 and claudin-3 in duodenal mucosa was lowest in NAFLD. On principal co-ordinate analysis (PCoA), the global bacterial composition was significantly different across the three groups (PERMANOVA test, P < 0.001).

Conclusion: While remaining activated in both etiologies, gut-barrier dysfunction abnormalities were more pronounced in NAFLD at early stages compared to ALD despite more advanced disease in the latter.

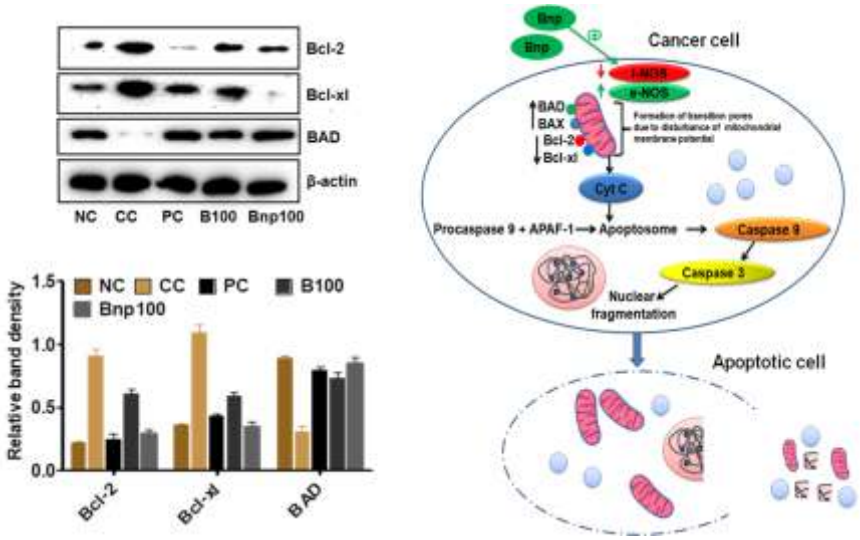


Caption: Comparison showing increased gut permeability and inflammation in NAFLD group compared to control and alcoholic CLD group.

Mechanistic exploration of the activities of PLGA-loaded betulinic acid nanoparticles against hepatocellular carcinoma at cellular and molecular levels

Pranesh Kumar, Anurag Kumar Gautam, Umesh Kumar, Archana S Bhadauria, Ashok K Singh, Dinesh Kumar, Tarun Mahata, Biswanath Maity, Hriday Bera, Sudipta Saha (2022). ***Archives of Physiology and Biochemistry***, 128 (3): 836-848

The effectiveness of betulinic acid (B) and PLGA loaded nanoparticles of B (Bnp) against hepatocellular carcinoma (HCC) was established and reported earlier. In continuation of our previous report, the present study described the molecular mechanisms of their antineoplastic responses. In this context, the antineoplastic properties of both B and Bnp were evaluated on DEN-induced HCC rat model. The quantitative real-time polymerase chain reaction and western blot analyses revealed that HCC was developed through lower expressions of e-NOS, BAX, BAD, Cyt C and higher expressions of i-NOS, Bcl-xl, Bcl-2. B and Bnpnormalised the expressions of these apoptogenic markers. Particularly, both activated i-NOS and e-NOS mediated Bcl-2 family proteins→CytC→Caspase 3 and 9 signalling cascades. The ^{1}H-NMR-based metabolomics study also demonstrated that the perturbed metabolites in DEN-induced rat serum restored to the normal level following both treatments. Moreover, the antineoplastic potential of Bnp was found to be comparable with the marketed product, 5-flurouracil.

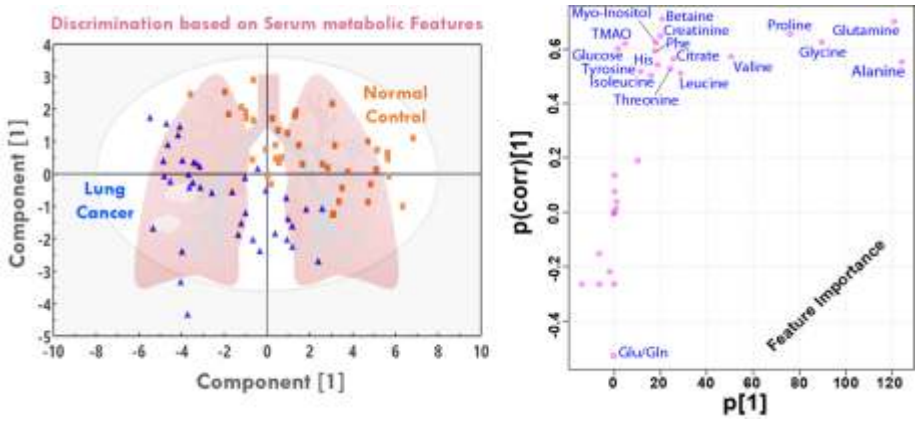


Proposed mechanism for the preclinical efficacy of PLGA loaded Bnp against hepatocellular carcinoma

Serum metabolic disturbances in lung cancer investigated through an elaborative NMR based serum metabolomics approach

Anjana Singh, Ved Prakash, Nikhil Gupta, Ashish Kumar, Ravi Kant, and Dinesh Kumar (2022). ***ACS Omega***, 7 (6): 5510–5520

Detection of metabolic disturbances in lung cancer (LC) has the potential to aid early diagnosis/prognosis and hence improve disease management strategies through reliable grading, staging, and determination of neoadjuvant status in LC. However, a majority of previous metabolomics studies compare the normalized spectral features which not only provide ambiguous information but further limit the clinical translation of this information. Various such issues can be resolved by performing the concentration profiling of various metabolites with respect to formate as an internal reference using commercial software Chenomx. Continuing our efforts in this direction, the serum metabolic profiles were measured on 39 LC patients and 42 normal controls (NCs, comparable in age/sex) using high-field 800 MHz NMR spectroscopy and compared using multivariate statistical analysis tools to identify metabolic disturbances and metabolites of diagnostic potential. Partial least-squares discriminant analysis (PLS-DA) model revealed a distinct separation between LC and NC groups and resulted in excellent discriminatory ability with the area under the receiver-operating characteristic (AUROC) = 0.97 [95% CI = 0.89–1.00]. The metabolic features contributing to the differentiation of LC from NC samples were identified first using variable importance in projection (VIP) score analysis and then checked for their statistical significance (with p-value < 0.05) and diagnostic potential using the ROC curve analysis. The analysis revealed relevant metabolic disturbances associated with LC. Among various circulatory metabolites, six metabolites, including histidine, glutamine, glycine, threonine, alanine, and valine, were found to be of apposite diagnostic potential for clinical implications. These metabolic alterations indicated altered glucose metabolism, aberrant fatty acid synthesis, and augmented utilization of various amino acids including active glutaminolysis in LC.

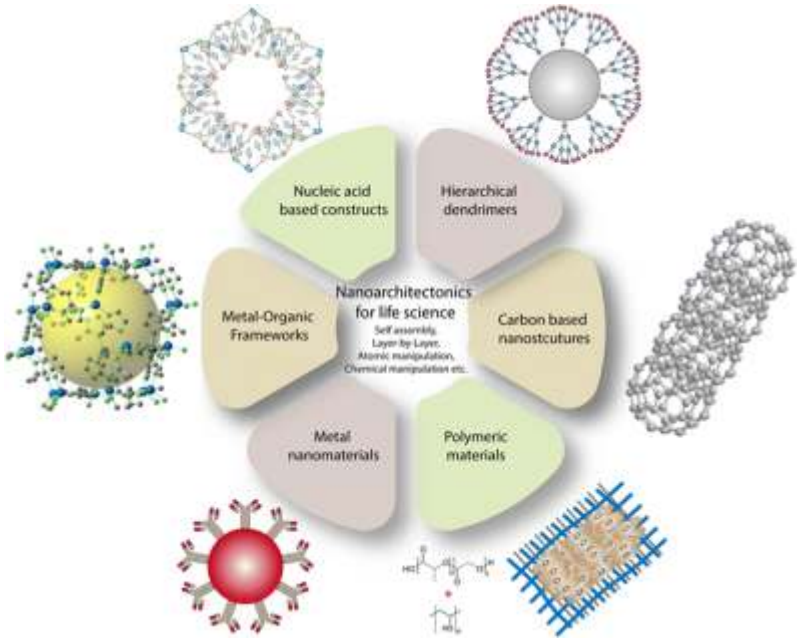


Multivariate analysis showing serum metabolic disturbances in lung cancer.

Nanoarchitectonics horizons: materials for life sciences

V. Karthick, Lok Kumar Shrestha, V. Ganesh Kumar, Pranjali Pranjali, Dinesh Kumar, Aniruddha Pal, Katsuhiko Ariga (2022). ***Nanoscale***, 14 (30): 10630-10647.

Nanoarchitectonics relies on the fabrication of materials at the atomic/molecular level to achieve the desired shape and function. Significant advances have been made in understanding the characteristics and spatial assemblies that contribute to material performance. Biomaterials undergo several changes when presented with various environmental cues. The ability to overcome such challenges, maintaining the integrity and effective functioning of native properties, can be regarded as a characteristic of a successful biomaterial. Control over the shape and efficacy of target materials can be tailored via various processes, like self-assembly, supramolecular chemistry, atomic/molecular manipulation, etc. Interplay between the physicochemical properties of materials and biomolecule recognition sites defines the structural rigidity in hierarchical structures. Materials including polymers, metal nanoparticles, nucleic acid systems, metal–organic frameworks, and carbon-based nanostructures can be viewed as promising prospects for developing biocompatible systems. This review discusses recent advances relating to such biomaterials for life science applications, where nanoarchitectonics plays a decisive role either directly or indirectly.



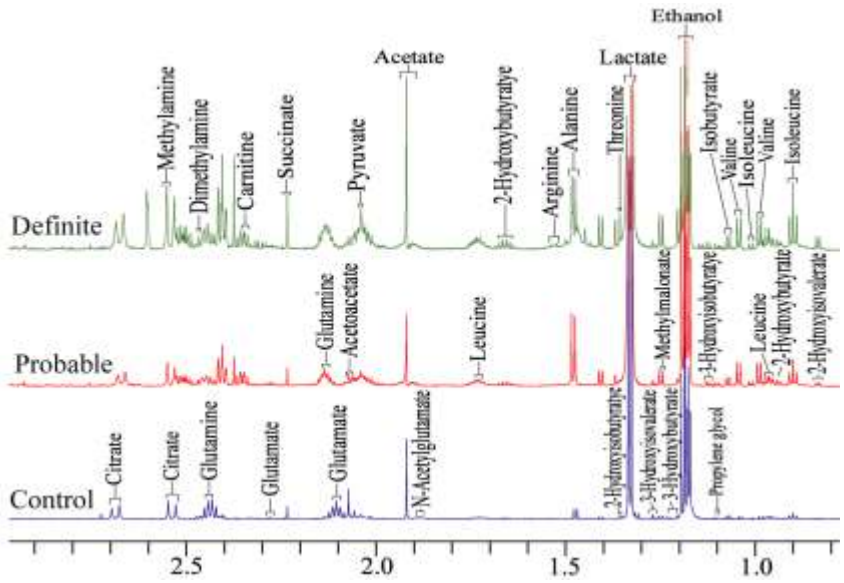
Prospects for developing biomaterials for life science applications via the nanoarchitectonics concept.

NMR based CSF metabolomics in tuberculous meningitis: correlation with clinical and MRI findings

Rashmi Parihar, Ruchi Shukla, Bikash Baishya, Jayantee Kalita, Rudrasish Haldar, Usha Kant Misra
(2022). ***Metabolic Brain Disease***, 37: 773 – 785

Although tuberculous meningitis (TBM) represents just 1% of all TB cases, it is the most lethal form of CNS(Central Nervous System) tuberculosis with an incidence of 30% mortality despite antitubercular treatment and neurological sequelae in about 50% of survivors. Early diagnosis is critical for improved clinical outcome, which is challenging due to the varied and nonspecific clinical presentations coupled to the low sensitivity and specificity of the existing diagnostic tests. For instance, mycobacterium culture is time consuming while Ziehl-Neelsen staining has a low detection rate.

Mycobacterium tuberculosis (Mtb) utilizes host cell metabolites and acquires specific metabolic pathways to use newly acquired substrate. Therefore, bio-molecular techniques could greatly aid early diagnosis by detecting metabolites which are significantly perturbed in TBM relative to control. We investigated the potential of ^{1}H NMR based metabolomics in TBM and correlated that to the other clinical-radiological parameters. Forty-three patients with TBM diagnosed based on clinical, CSF, and MRI were included. The severity of meningitis was categorized as stages I, II, and III. Furthermore, the patients with either positive for Mtb or PCR for Mtb were considered definite. ^{1}H NMR based metabolomics detected 11 metabolites which could distinguish TBM from the controls. In TBM, lactate, glutamate, alanine, arginine, 2-hydroxyisobutyrate, formate, and cis-aconitate were upregulated, and glucose, fructose, glutamine, and myo-inositol were downregulated compared to the controls. In the ROC analysis these metabolites were able to classify cases with good sensitivity and specificity. Increased CSF glutamate and decreased glutamine levels, and enhanced arginine has a role in cognitive and motor function decline in TBM.

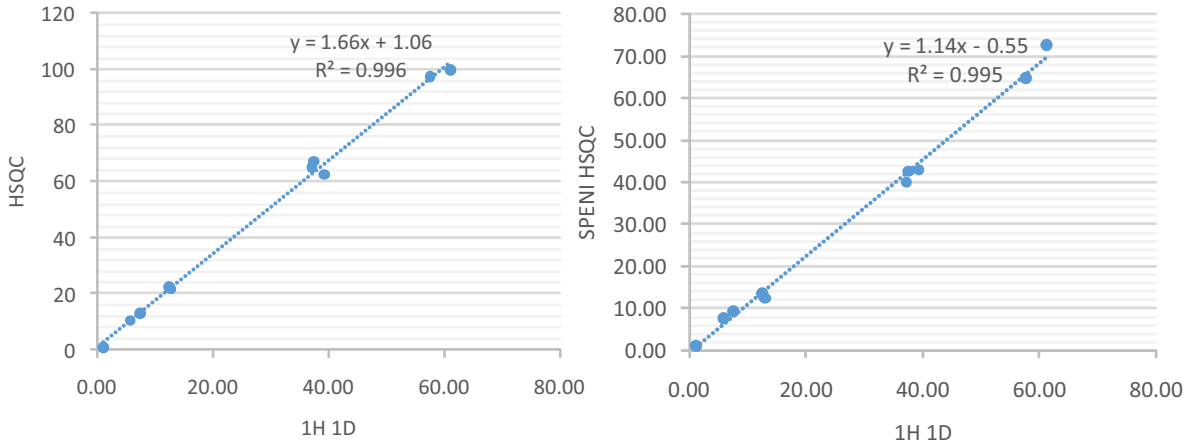


Stack plot of cumulative 1D 1H NMR spectra (selected region displayed) of CSF samples showing region (A) δ0.8 to 2.9 ppm and for definite TBM, probable TBM, and healthy controls respectively.

Spatially Encoded Polarization Transfer for Improving the Quantitative Aspect of ^{1}H-^{13}C HSQC

Bikash Baishya, Rajeev verma, Rashmi Parihar (2022). ***Journal of Magnetic Resonance Open***, 12-13: 100063

One-dimensional (1D) ^{1}H NMR is routinely used for metabolomics studies. However, 1D ^{1}H NMR displays significant spectral overlap. Peak overlap is minimized by 2D ^{1}H -^{13}C HSQC spectrum due to the presence of two dimensions. Therefore, 2D HSQC has the potential to open new avenues for following metabolism in biological systems in which 1D ^{1}H NMR is limited by signal overlap. However, the quantification aspect of HSQC is not straightforward. The variations in ^{1}H-^{13}C scalar couplings, T_1, T_2, and pulse imperfections contribute to this problem in 2D HSQC. Although T_1, T_2 can be suitably chosen to minimize their deleterious effects, the differential polarization transfer for different resonances owing to large variations in ^{1}H -^{13}C couplings does not allow the cross-peak intensities to be directly correlated to the quantity of metabolites. We have developed a spatial encoding strategy in which we show that spatial encoding of the ^{1}H to ^{13}C polarization transfer delays in HSQC using sweep frequency pulses in the presence of magnetic field gradient allows one to perform a uniform transfer of polarization from ^{1}H to ^{13}C over a range of ^{1}H -^{13}C couplings improving the quantitative aspect of HSQC. We show that in this new technique- SPENI HSQC a variable *J*-evolution period can be imparted during polarization transfer steps within a single scan which otherwise needs multiple scans and iterative optimization. This method will broaden the scope of 2D NMR for quantification of complex mixtures crucial in metabolomics.

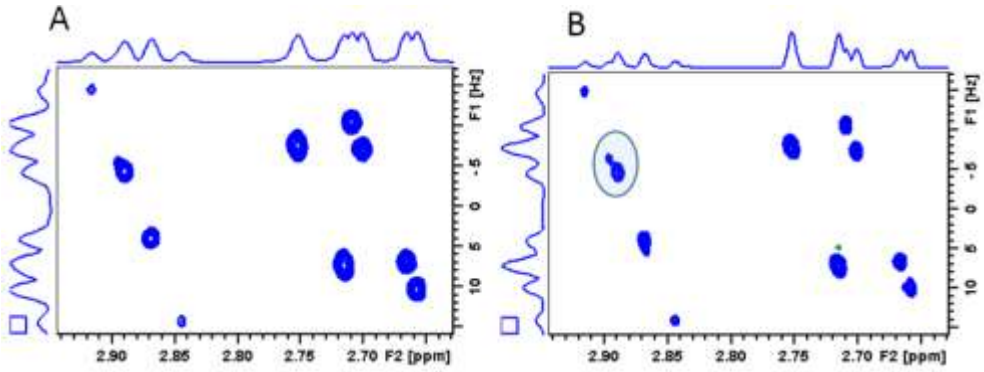


A & B are regression curves of the integrals obtained from regular HSQC and SPENI HSQC, respectively, when plotted vs. ^{1}D ^{1}H NMR integrals. The solvent signal (0.2% CHC^{l3}) was normalized to 1 in the ^{1}H ^{1}D and also in all HSQC. The bar plot in Fig 4A shows that regular HSQC overestimates all integral values relative to ^{1}H ^{1}D, and likewise, the regression curve deviates significantly from ^{1}H ^{1}D NMR, y=1.66x. The SPENI-HSQC displays a much better correlation of its integrals to ^{1}H ^{1}D integral values (Fig B) and a regression curve y=1.14x with only 14% deviations from the 1:1 correspondence with ^{1}H NMR.

Slice Selective Absorption-Mode J-Resolved NMR Spectroscopy (SS J-RES Spectroscopy)

Bikash Baishya (2022). ***Journal of Magnetic Resonance***, 342: 107267

Limited chemical shift dispersion and broad multiplet patterns can limit the application of ^{1}H NMR spectra. J-Resolved spectroscopy of protons improve resolution by reducing signal overlap issues in complex ^{1}H spectra. However, the phase-twist line shape in J-Resolved spectroscopy allows only the magnitude mode of the experiment to be practical, which degrades resolution. Recently, various pure shift or broadband homonuclear decoupling approaches have been integrated with J-Resolved spectroscopy to eliminate the broad dispersive contribution. In this direction, we developed a simple and effective procedure- SS J-RES spectroscopy for recording broadband ^{1}H-^{1}H J-Resolved spectrum with greatly reduced dispersive contribution to the lineshape which otherwise reduces resolution of the signals. This we did using the concept of slice selection that employs weak rf pulses in the presence of weak magnetic field gradient. We show that slice selective excitation, t_1 encoding, storage, and detection of the in-phase absorptive signals can be executed, while a gradient-based suppression of the dispersive antiphase signals can be performed. Further, the fresh magnetization from neighboring slices can be accessed in different scans by frequency shifting of the slice selective pulses without a recycle delay. This allows faster signal averaging, improving sensitivity which depends on the T_1 relaxation time of the signals. This method displays sensitivity up to 4-20 percent of the regular J-RES ^{1}H signals while at the same time also provides a superior resolution.

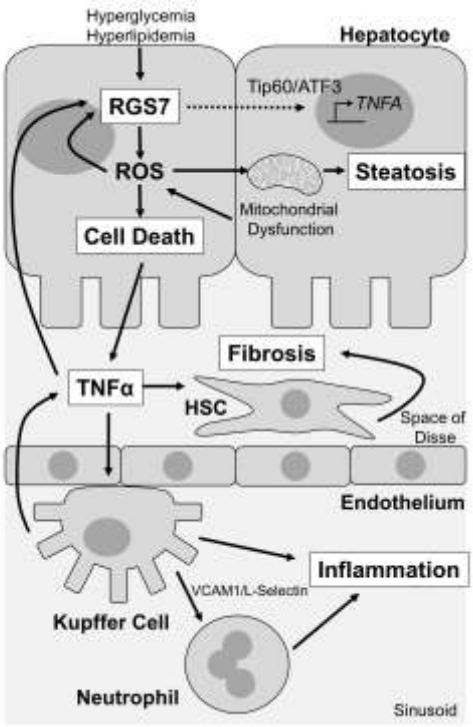


Expanded portion of regular magnitude mode J-RES (A) and absorptive mode SS J-RES spectrum (B) for a few selected peaks (plotted on the same contour levels) recorded on a sample of strychnine. Narrow lineshape and improved resolution are evident in the absorptive BS J-RES spectrum (B).

RGS7-ATF3-Tip60 Complex Promotes Hepatic Steatosis and Fibrosis by Directly Inducing TNFa

Madhuri Basak,Kiran Das,Tarun Mahata,Abhishek Singh Sengar,Sumit Kumar Verma,Sayan Biswas,Kakali Bhadra,Adele Stewart, Biswanath Maity (2022). ***Antioxidants & Redox Signaling***, 38 (1-3): 137-159.

The pathophysiological mechanism(s) underlying non-alcoholic fatty liver disease (NAFLD) have yet to be fully delineated and only a single drug, peroxisome proliferator-activated receptor (PPAR) a/c agonist saroglitazar, has been approved. Here, we sought to investigate the role of Regulator of G Protein Signaling (RGS7) in hyperlipidemia-dependent hepatic dysfunction. RGS7 is elevated in the livers of NAFLD patients, particularly those with severe hepatic damage, pronounced insulin resistance, and high inflammation. In the liver, RGS7 forms a unique complex with transcription factor ATF3 and histone acetyltransferase Tip60, which is implicated in NAFLD. The removal of domains is necessary for ATF3/Tip60 binding compromises RGS7-dependent reactive oxygen species generation and cell death. Hepatic RGS7 knockdown (KD) prevented ATF3/Tip60 induction, and it provided protection against fibrotic remodeling and inflammation in high-fat diet-fed mice translating to improvements in liver function. Hyperlipidemia-dependent oxidative stress and metabolic dysfunction were largely reversed in RGS7 KD mice. Interestingly, saroglitazar failed to prevent RGS7/ATF3 upregulation but it did partially restore Tip60 levels. RGS7 drives the release of particularly tumor necrosis factor a (TNFa) from isolated hepatocytes, stellate cells and its depletion reverses steatosis, oxidative stress by direct TNFa exposure. Conversely, RGS7 overexpression in the liver is sufficient to trigger oxidative stress in hepatocytes that can be mitigated via TNFa inhibition. We discovered a novel non-canonical function for an R7RGS protein, which usually functions to regulate G protein coupled receptor (GPCR) signaling. This is the first demonstration for a functional role of RGS7 outside the retina and central nervous system. RGS7 represents a potential novel target for the amelioration of NAFLD.

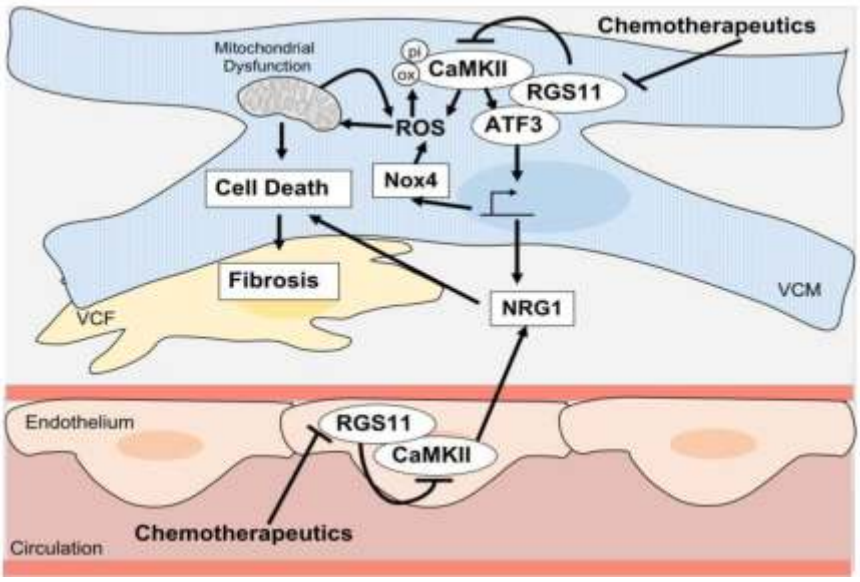


RGS7 promotes liver fibrosis by regulating TNFa

RGS11-CaMKII complex mediated redox control attenuates chemotherapy-induced cardiac fibrosis

Kiran Das, Madhuri Basak, Tarun Mahata, Manish Kumar, Dinesh Kumar, Sayan Biswas, Suvro Chatterjee, Mahammed Moniruzzam, Nimai Chandra Saha, Kausik Mondal, Pranesh Kumar, Priyadip Das, Adele Stewart, Biswanath Maity (2022). ***Redox Biology***, 57: 102487

Dose limiting cardiotoxicity remains a major limiting factor in the clinical use of several cancer chemotherapeutics including anthracyclines and the antimetabolite 5-fluorouracil (5-FU). Prior work has demonstrated that chemotherapeutics increase expression of R7 family regulator of G protein signaling (RGS) protein-binding partner Gβ5, which drives myocyte cytotoxicity. However, though several R7 family members are expressed in heart, the exact role of each protein in chemotherapy driven heart damage remains unclear. Here, we demonstrate that RGS11, downregulated in the human heart following chemotherapy exposure, possesses potent antiapoptotic actions, in direct opposition to the actions of fellow R7 family member RGS6. RGS11 forms a direct complex with the apoptotic kinase CaMKII and stress responsive transcription factor ATF3 and acts to counterbalance the ability of CaMKII and ATF3 to trigger oxidative stress, mitochondrial dysfunction, cell death, and release of the cardiokine neuregulin-1 (NRG1), which mediates pathological intercommunication between myocytes and endothelial cells. Doxorubicin triggers RGS11 depletion in the murine myocardium, and cardiac specific OE of RGS11 decreases doxorubicin-induced fibrosis, myocyte hypertrophy, apoptosis, oxidative stress, and cell loss and aids in the maintenance of left ventricular function. Conversely, RGS11 knockdown in heart promotes cardiac fibrosis associated with CaMKII activation and ATF3/NRG1 induction. Indeed, inhibition of CaMKII largely prevents the fibrotic remodeling resulting from cardiac RGS11 depletion underscoring the functional importance of the RGS11-CaMKII interaction in the pathogenesis of cardiac fibrosis. These data describe an entirely new role for RGS11 in heart and identify RGS11 as a potential new target for amelioration of chemotherapy-induced cardiotoxicity.

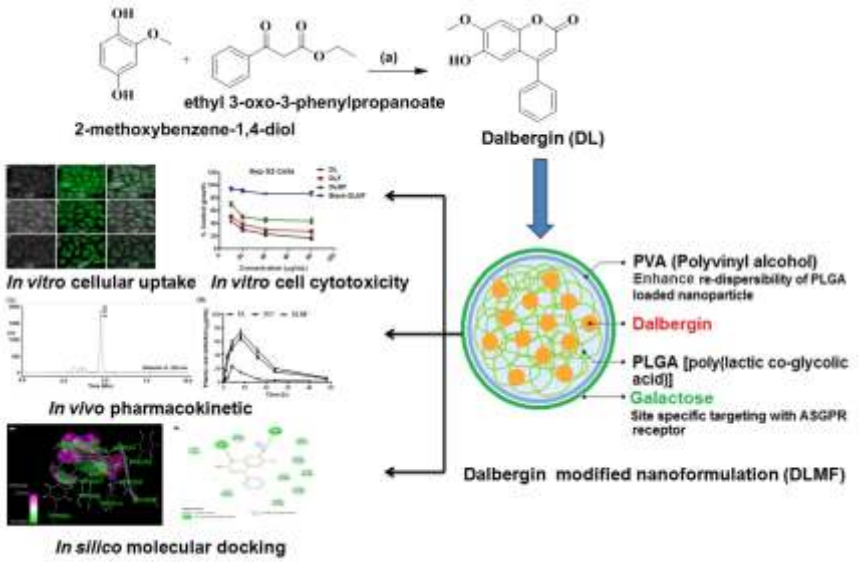


RGS11 functions to limit chemo-induced cardiac pathologies

Synthesis and appraisal of dalbergin-loaded PLGA nanoparticles modified with galactose against hepatocellular carcinoma: *In-vitro*, pharmacokinetic, and *in-silico* studies

Anurag Kumar Gautam, Pranesh Kumar, Biswanath Maity, Ganesh Routholla, Balaram Ghosh, Kumarappan Chidambaram, M Yasmin Begum, Adel Al Fatease, P S Rajinikanth, Sanjay Singh, Sudipta Saha, Vijayakumar M R (2022). ***Frontiers in Pharmacology***, 13:1021867.

Hepatocellular carcinoma (HCC) is a common malignancy which affects a substantial number of individuals all over the globe. It is the third primary cause of death among persons with neoplasm and has the fifth largest mortality rate among men and the seventh highest mortality rate among women. Dalbergin (DL) is described to be effective in breast cancer via changing mRNA levels of apoptosis-related proteins. DL belongs to neoflavonoids, a drug category with low solubility and poor bioavailability. We created a synthetic version of this naturally occurring chemical, DL, and then analyzed it using 1H-NMR, 13C-NMR, and LC-MS. We also made PLGA nanoparticles and then coated them with galactose. The design of experiment software was used to optimize DL-loaded galactose-modified PLGA nanoparticles. The optimized DL-nanoformulations (DLF) and DL-modified nanoformulations (DLMF) were analyzed for particle size, polydispersity index, shape, and potential interactions. In-vitro experiments on liver cancer cell lines (HepG2) are used to validate the anti-proliferative efficacy of the modified DLMF. The in-vitro research on HepG2 cell lines also demonstrated cellular accumulation of DLF and DLMF by FITC level. The in-vitro result suggested that DLMF has high therapeutic effectiveness against HCC. In-vivo pharmacokinetics and bio-distribution experiments revealed that DLMF excelled pristine DL in terms of pharmacokinetic performance and targeted delivery, which is related to galactose's targeting activity on the asialoglycoprotein receptor (ASGPR) in hepatic cells. Additionally, we performed an in-silico study of DL on caspase 3 and 9 proteins, and the results were found to be −6.7 kcal/mol and −6.6 kcal/mol, respectively. Our in-silico analysis revealed that the DL had strong apoptotic properties against HCC.

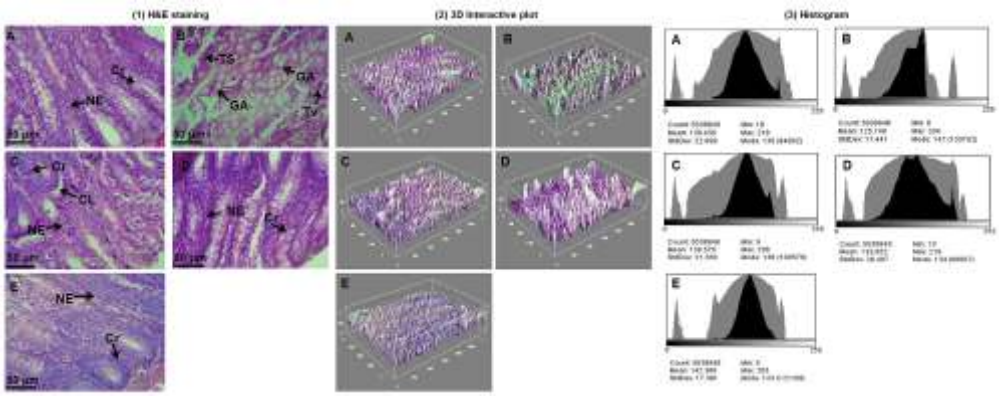


Dalbargin nano particle blocks liver cancer

Preclinical Evaluation of Dimethyl Itaconate Against Hepatocellular Carcinoma via Activation of the e/iNOS-Mediated NF-κB-Dependent Apoptotic Pathway

Anurag Kumar Gautam, Pranesh Kumar, Ritu Raj, Dinesh Kumar, Bolay Bhattacharya, P.S. Rajinikanth, Kumarappan Chidambaram, Tarun Mahata, Biswanath Maity, and Sudipta Saha (2022). ***Frontiers in Pharmacology***, 12: 823285.

Hepatocellular carcinoma (HCC) is one of the most common tumors affecting a large population worldwide, with the fifth and seventh greatest mortality rates among men and women, respectively, and the third prime cause of mortality among cancer victims. Dimethyl itaconate (DI) has been reported to be efficacious in colorectal cancer by decreasing IL-1β release from intestinal epithelial cells. In this study, diethylnitrosamine (DEN)-induced HCC in male albino Wistar rats was treated with DI as an anticancer drug. The function and molecular mechanism of DI against HCC in vivo were assessed using histopathology, enzyme-linked immunosorbent assay (ELISA), and Western blot studies. Metabolomics using 1H-NMR was used to investigate metabolic profiles. As per molecular insights, DI has the ability to trigger mitochondrial apoptosis through iNOS- and eNOS-induced activation of the NF-κB/Bcl-2 family of proteins, CytC, caspase-3, and caspase-9 signaling cascade. Serum metabolomics investigations using 1H-NMR revealed that aberrant metabolites in DEN-induced HCC rats were restored to normal following DI therapy. Furthermore, our data revealed that the DI worked as an anti-HCC agent. The anticancer activity of DI was shown to be equivalent to that of the commercial chemotherapeutic drug 5-fluorouracil.

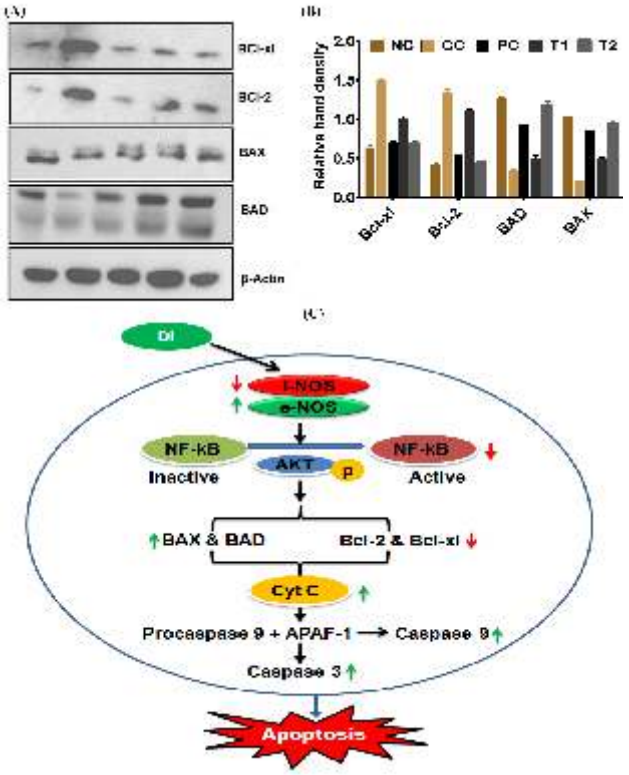


RGS7 drives DI attenuates liver cancer phenotype

Ameliorative effect of fluvoxamine against colon carcinogenesis via COX-2 blockade with oxidative and metabolic stress reduction at the cellular, molecular and metabolic levels

Pranesh Kumar, Mohit kumar, Anurag Kumar Gautam, Archana Bharti Sonkar, Abhishek Verma, Amita Singh, Raquibun Nisha, Umesh Kumar, Dinesh Kumar, Tarun Mahata, Bolay Bhattacharya, Biswanath Maity, Abhishek Pandeya, Sunil Babu Gosipatala, Sudipta Saha (2022). ***BBA Advances***, 2: 100046.

Fluvoxamine's (FLX's) anticancer potential was investigated in pre-clinical research utilizing a DMH-induced colorectal cancer (CRC) rat model. qRT-PCR and immunoblotting validated the mechanistic investigation. The CRC condition was induced in response to COX-2 and IL-6, however, following FLX therapy, the condition returned to normal. FLX's anti-CRC potential may be attributable to COX-2 inhibition since this molecular activity was more apparent for COX-2 than IL-6. FLX repaired the altered metabolites linked to CRC rats, according to 1H-NMR analysis. FLX was shown to be similar to 5-FU in terms of tumor protection, which may be useful in future medication development.

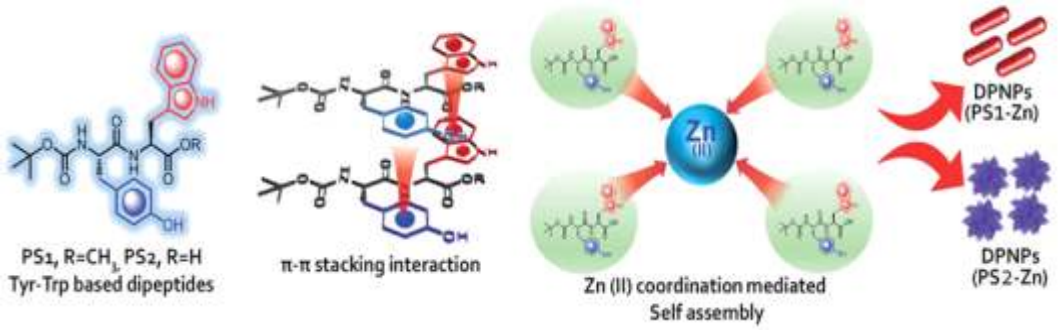


Fluvoxamine prevents colon cancer

Self-assembled dipeptide based fluorescent nanoparticles as a platform for developing cellular imaging probes and targeted drug delivery chaperones

Subramaniyam Sivagnanam, Kiran Das, Madhuri Basak, Tarun Mahata, Adele Stewart, Biswanath Maity, Priyadip Das (2022). ***Nanoscale Advances***, 4 (6): 1694-1706.

Self-assembled peptide-based nanostructures, comprised of naturally occurring amino acids, display excellent biocompatibility, biodegradability, flexible responsiveness, and synthetic feasibility and can be customized for various biomedical applications. However, the lack of inherent optical properties of peptide-based nanoparticles is a limitation on their use as imaging probes or drug delivery vehicles. To overcome this impediment, we generated Boc protected tyrosine–tryptophan dipeptide-based nanoparticles (DPNPs) with structure rigidification by Zn(II), which shifted the peptide's intrinsic fluorescent properties from the ultraviolet to the visible range. These DPNPs are photostable, biocompatible and have visible fluorescence signals that allow for real-time monitoring of their entry into cells. We further show that two DPNPs (PS1-Zn and PS2-Zn) can encapsulate the chemotherapeutic drug doxorubicin (Dox) and facilitate intracellular drug delivery resulting in cancer cell killing actions comparable to the unencapsulated drug. Finally, we chemically modified our DPNPs with an aptamer directed toward the epithelial cell surface marker EPCAM, which improved Dox delivery to the lung cancer epithelial cell line A549. In contrast, the aptamer conjugated DPNPs failed to deliver Dox into the cardiomyocyte cell line AC16. Theoretically, this strategy could be employed in vivo to specifically deliver Dox to cancer cells while sparing the myocardium, a major source of dose-limiting adverse events in the clinic. Our work represents an important proof-of-concept exercise demonstrating that ultra-short peptide-based fluorescent nanostructures have great promise for the development of new imaging probes and targeted drug delivery vehicles.

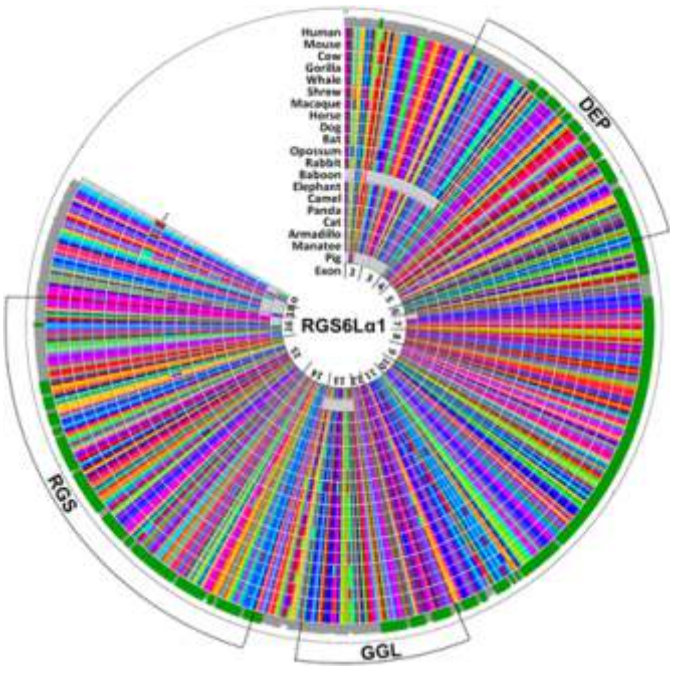


Dipeptide based nanoparticles as a platform for drug delivery

Protein profiling of RGS6, a pleiotropic gene implicated in numerous neuropsychiatric disorders, reveals multi-isoformic expression and a novel brain-specific isoform

K E Ahlers-Dannen, J Yang, M M Spicer, B Maity, A Stewart, J G Koland, R A Fisher (2022). ***eNeuro***, 9 (1).

A metanalysis identified Regulator of G protein Signaling 6 (RGS6) as one of 23 loci with pleiotropic effects on four or more human psychiatric disorders. This finding is significant as it confirms/extends the findings of numerous other studies implicating RGS6 in CNS function and pathology. RGS6 is a highly conserved member of the RGS protein family whose cellular roles are likely affected by mRNA splicing and alternative domain inclusion/exclusion. Indeed, we previously identified multiple RGS6 splice variants predicted to produce 36 distinct protein isoforms containing either long (RGS6L) or short (RGS6S) N-terminal domains, an incomplete or intact GGL domain, and 9 alternative C-termini. Unfortunately, sequence similarities between the isoforms have made it difficult to confirm their individual existence and/or to determine their unique functions. Here, we developed 3 RGS6-specific antibodies that recognize all RGS6 protein isoforms (RGS6-fl), the N-terminus of RGS6L isoforms (RGS6-L), and an 18 amino acid alternate C-terminal sequence (RGS6-18). Using these antibodies, we demonstrate that RGS6L(+GGL) isoforms, predominating in both mouse (both sexes) CNS and peripheral tissues, are most highly expressed in the CNS. We further identify 3 novel RGS6 protein bands that are larger (61, 65, and 69kDa) than the ubiquitously expressed 53-57kDa RGS6L(+GGL) proteins. Importantly, we show that the 69kDa protein is a brain-specific dephospho- form of the 65 kDa band, the first identified phosphorylated RGS6 isoform. Together, these data begin to define the functional significance behind the complexity of RGS6 gene processing and further clarifies RGS6's physiological roles by resolving tissue-specific RGS6 protein expression.

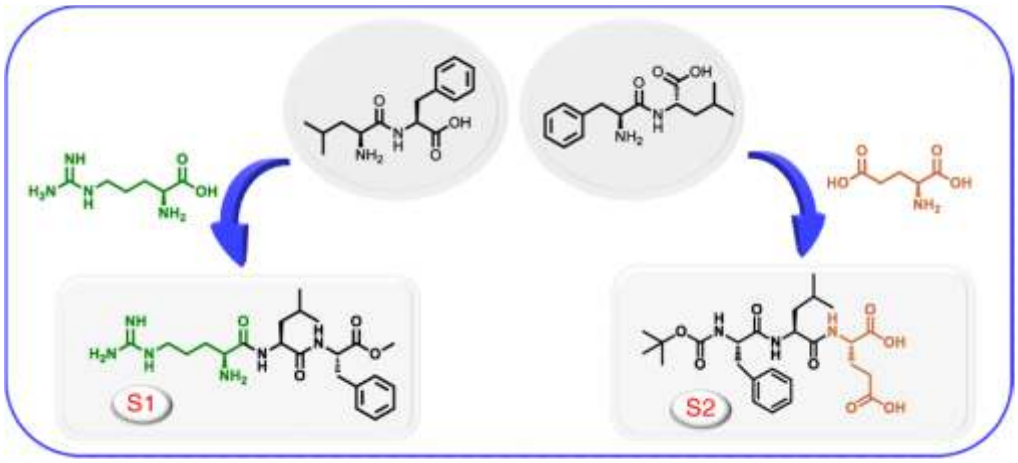


RGS6 protein implicated in neuropsychiatric diseases

Generation of Self-Assembled Structures Composed of Amphipathic, Charged Tripeptides for Intracellular Delivery of Pro-Apoptotic Chemotherapeutics

Subramaniyam Sivagnanam, Kiran Das, Vijay Sivakadatcham, Tarun Mahata, Madhuri Basak, Ieshita Pan, Adele Stewart, Biswanath Maity, Priyadip Das (2022). ***Israel Journal of Chemistry***, 62 (9-10): e202200001.

Chemotherapeutic drugs remain the most efficacious treatment options for a many human cancers. However, the inability to deliver these drugs directly to cancerous cells often results in dose limiting and sometimes life-threatening adverse effects. Rather than developing new chemical moieties, researchers have begun focusing on the development of drug carriers, which are specifically designed to shuttle chemotherapeutics into malignant cells while sparing healthy cells. Charged nanoparticles have emerged as effective delivery platforms for several xenobiotic classes including anticancer agents, oligonucleotides and antibodies. Notably, peptide-based self-assembled nanostructures are of particular interest due to their biocompatibility, high drug loading capacity, and potential for customization for cell specific targeting. We synthesized and studied the self assembling properties of two charged, cell penetrating tripeptides with Glu as negatively charged amino acid. The fibrils and spherical self assembled structures formed by S1 and S2, respectively, can encapsulate the chemotherapeutic drug Doxorubicin and facilitate intracellular drug delivery via endocytosis. Furthermore, S1- and S2-encapsulated Doxorubicin (Dox-S1, Dox- S2), like the unencapsulated drug, induced oxidative stress and mitochondrial dysfunction, activated the ATM/p53 signaling cascades, and triggered apoptosis in cancer cells. Thus, while the surface charge of molecular building blocks used to generate supramolecular assemblies influences the morphology of generated nanostructures, both cationic and anionic peptide-based assemblies are capable of functioning as drug delivery vehicles.

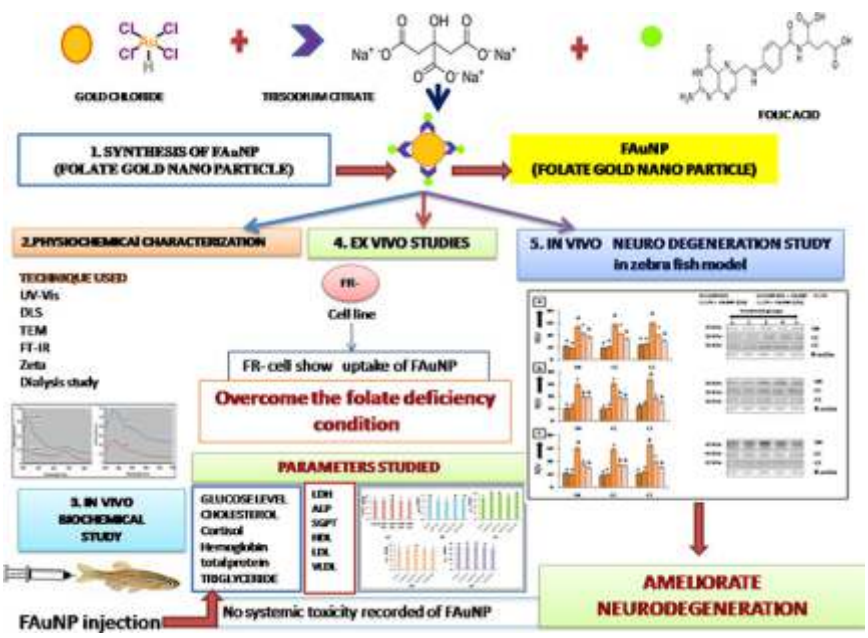


Self assembled structures for intracellular delivery

Organometallic Folate Gold Nanoparticles Ameliorate Lipopolysaccharide-Induced Oxidative Damage and Inflammation in Zebrafish Brain

Susanta Sadhukhan, Mahammed Moniruzzaman, Subhajit Maity, Sudakshina Ghosh, Arup Kumar Pattanayak, Suman Bhusan Chakraborty, Biswanath Maity, Madhusudan Das (2022). ***ACS Omega***, 7 (11): 9917 – 9928.

Synthesized organometallic gold-based folate nanoparticles (FAuNPs) were characterized, and its defense against lipopolysaccharide (LPS)-induced brain inflammation in Zebra fish was proven. Vitamin entrapment efficiency of these particles was found to be nearly 70%. The in vitro pH-dependent drug release dialysis study of FAuNPs confirmed a slow, sustained, and gradual release of folate for a period of 24 h. Both AuNPs and FAuNPs did not cause any marked changes in food intake, body weight, color, behavioral pattern, blood parameters, and hepatotoxicity. Histology of liver showed no changes between treated and control groups of fishes. The ex vivo study showed significant uptake of FAuNPs to free folate in folate receptor negative Hek293 cells, confirming a strategy to overcome folate deficiency in the brain. Antioxidant status and activities of few crucial brain enzymes were also measured to assess the brain function and found to be returned to the basal level, following FAuNP treatment. The transcription factor NRF2-Keap 1 expression pattern was also noted, and a prominent modulation was observed in the LPS-treated and FAuNP-administered group. Decisive brain enzymes like AChE and Na+K+ATPase were decreased significantly after LPS treatment, which is restored with FAuNP treatment. Caspases increased sharply after LPS treatment and diminished following FAuNP treatment. We conclude that FAuNP due to its high physical stability and uptake could be utilized against severe brain inflammation, leading to brain injury and neurodegeneration.



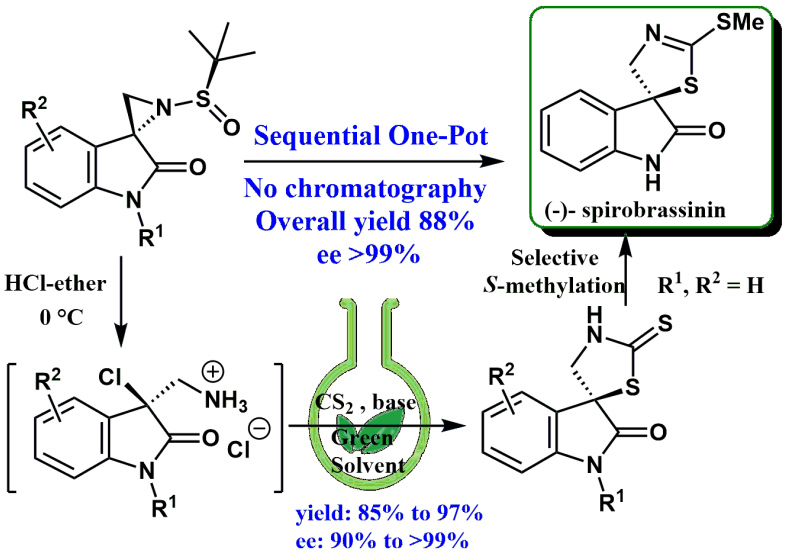
Nanoparticles regulate inflammation in fish brain

Regio- and Stereospecific Desulfinylative Chlorination of Spiroaziridine Oxindoles at Spiro-Center for Formal [3+2]-Cycloaddition with CS_2: Sequential One-Pot Synthesis of (-)-Spirobrassinin

Anurag Biswas and Saumen Hajra
(2022). ***Advanced Synthesis & Catalysis***, 364: 3035-3042.

Phytoalxeins are naturally produced in defense metabolisms within diseased plant cells when exposed to radiation, heavy metalpoisoning or pathogenic activity. In past few decades, numerous biological studies with phytoalxeins, particularly, (*S*)-(-)-spirobrassinin, revealed a broad range of activities, such as anti-microbial, chemopreventive, antitumor, anti-trypanosomal, anti-aggregation. Hence, synthesis of such crucial scaffold had been a keen interest to several groups. However, maintaining high enantiopurity as well as yield, is still a major challenge. The scalable asymmetric synthesis of spirobrassinin and its analogues with high enantiopurity is in demand and still an unmet challenge.

We have developed a HCl-promoted desulfinylative chlorination of *N-tert*-butylsufinylspiroaziridine oxindoles and subsequent regio- and stereocontrolled formal [3+2]-cycloaddition with CS_2 for the successful construction of 2'-thioxospiro[indoline-3,5'-thiazolidin]-2-ones with excellent yield and enantiopurity. Significant value of the method has been depicted by a sequential one-pot scalable synthesis of highly enantiopure (>99% ee) naturally occurring phytoalexin, (-)-spirobrassinin. Moreover, experimental findings of the current method have strengthened the mechanistic overview on unique reactivity of 3-(aminomethyl)-3-chloro-indolin-2-one derived from spiroaziridine oxindoles in [3+2]-cycloaddition reactions.

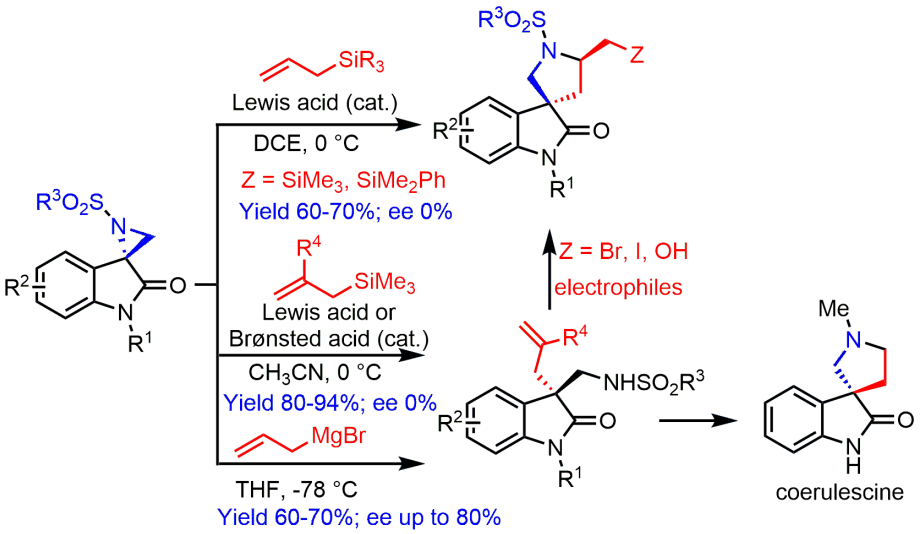


Selective C3-Allylation and Formal [3+2]-Annulation of Spiro-aziridine Oxindoles: Synthesis of 5^1 -Substituted Spiro[pyrrolidine-3,3′-oxindoles] and Coerulescine

SK Abu Saleh, Atanu Hazra, Maya Shankar Singh, Saumen Hajra
(2022). ***The Journal of Organic Chemistry***, 87 (13): 8656-8671.

The spirooxindole bearing azacycles gain intense attention from synthetic as well as medicinal chemistry due to their unique three-dimensional architecture and interesting biological profiles. Among them, 3,3′-pyrrolidinyl-spirooxindole is a privileged and most studied scaffold that defines the characteristics structural core in a large family of bioactive natural alkaloids and synthetic compounds often exhibit intriguing biological properties like anticancer, anti-tumor, anti-microbial, anti-viral, and antimalarial activities. The synthesis of architecturally fascinating spiro(pyrrolidinyloxindole) alkaloids such as coerulescine and horsfiline, bearing an all-carbon quaternary center at the C3-position of oxindole have attracted much attention over the past decades.

Spiroaziridine oxindole is the smallest spiro-aza-cycle of oxindoles and a new subgroup of aziridine has recently been developed and explored by our group as a brilliant building block to access several 3,3-disubstituted- and spiro-oxindole compounds and attracted the attention to others too. Brønsted acid and/or Lewis acid-catalyzed selective C3-allylation and formal [3+2]-annulation of spiro-aziridine oxindoles with allylsilanes have been demonstrated to deliver direct access to 3-allyl-3-aminomethyl oxindoles and 5-silyl methyl spiro[pyrrolidine-3,3′-oxindoles], respectively. The acid-catalyzed methods do not provide any stereoselectivity when chiral spiroaziridines are used. However, the reaction of non-racemic sprioaziridines with allyl-Grignard reagent under catalyst-free conditions afforded 3-allyl-3-aminomethyl oxindoles with good stereoselectivity (ee up to 80%). The allylation protocol is utilized for the short synthesis of coerulescine and various 5 -substituted spiro[pyrrolidine-3,3′-oxindoles].

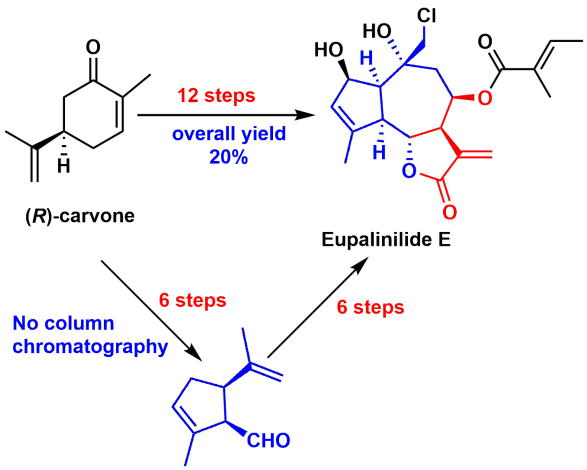


Asymmetric Total Synthesis of Eupalinilide E, a Promoter of Human HSPC Expansion

Ramkrishna Maity and Saumen Hajra (2022). ***Organic Letters***, 24 (26): 4745-4749.

Eupalinilide E, a sesquiterpene lactone, shows strong and selective cytotoxic activity against human lung cancer cell line A549 cells, which is known to harbor KRAS mutation, with an IC_{50} of 28 nM, but no activity against leukemia cell line P388 cells. There is a critical demand to develop drugs for this KRAS mutant non-small lung cancer. It is later found that eupalinilide E is a remarkable promoter for the expansion of hematopoietic stem and progenitor cells (HSPCs) that has the potential to improve the success of bone marrow transplants and the treatment of various blood diseases and disorders. Unfortunately, there is no approved drug/compound to date for the ex vivo and in vivo production of HSPCs. Thus, eupalinilide E could be a potential lead compound for the development drugs for KRAS mutant non-small lung cancer and a promoter of ex-vivo expansion of HSPCs. So, the biological importance of eupalinilide E and its natural scarcity demands the development of a concise and scalable approach to total synthesis that would enable further biological evaluation.

We have developed a concise and scalable total synthesis of eupalinilde E in 12 steps with an overall yield of 20% from commercially available (*R*)-(-)-carvone involving only six chromatographic purifications. In total synthesis, it always strives for new reactions which will deliver increasingly complex targets in short order that will lead to better targets and also to generate a large number of natural products like compounds with wide diversity. In this direction, to accomplish the total synthesis of eupalinilide E in shorter order, we have developed a new tandem Favorskii rearrangement and elimination reaction of O-acetyl/tosyl chlorohydrin derived from (*R*)-(-)-carvone to afford cyclopentenyl carboxylic acid derivatives that furnished the chromatography-free six-step efficient and scalable (100 g) synthesis of 2-cyclopentene carbaldehyde, a key precursor, from (*R*)-(-)-carvone with excellent regio- and stereoselectivity. Further, a catalyst-free stereospecific tandem allylboration-lactonization of newly designed allylboranates with 2-cyclopenete carbaldehyde derived from (*R*)-(-)-carvone is developed using trifluoroethanol (TFE) as a promoter and recyclable solvent, where the susceptibility of the b, g-unsatuated aldehyde toward isomerization under acidic, basic, as well as thermal conditions is efficiently overcome.The development of these new protocols not only led to a pot- and step economy synthesis of eupalinilide E achieving high overall yield (20%) but also reduces the bulk solvents uses in work up & purification and in turn diminish the waste production and the cost of synthesis.



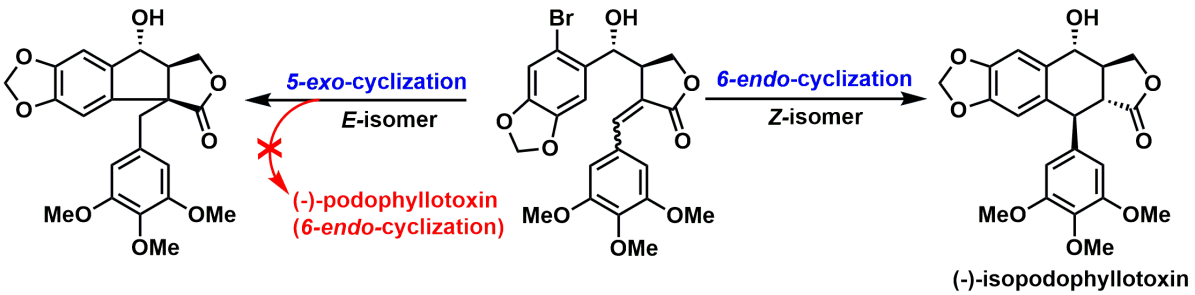
Stereochemistry of the Benzylidene - Butyrolactone Dictates the Reductive Heck Cyclization Mode in Asymmetric Synthesis of Aryltetralin Lignans: A Detail Experimental and Theoretical Study.

Biswajit Sen, Saikat Roy, Sujay Garai, Sayan Roy, Anakuthil Anoop and Saumen Hajra (2022). ***The Journal of Organic Chemistry***, 87 (6): 3910-3921.

Article on Cover Page

Among the wide variety of lignan natural products, aryltetralin lignans attract considerable attention to chemists and biologists since they possess a significant arsenal in the battle against human diseases and their study continues to unveil unexpected biological properties. Thus, a lot of synthetic chemists including our group are involved in the total synthesis of these classes of natural products, in particular (-)-podophyllotoxin. Earlier, we had completed the synthesis by utilizing intramolecular Heck cyclization followed by a solvent-controlled catalytic transfer hydrogenation (CTH) protocol for the synthesis of (-)-podophyllotoxindespite a moderate selectivity. To overcome this shortcoming and to reduce the usage of catalyst by curtail of steps, we wanted to revisit the synthesis again by utilizing the intramolecular reductive Heck cyclization instead of a two steps protocol.

The reductive Heck cyclization of non-racemic benzylidene -butyrolactone is studied towards asymmetric synthesis of aryltetralin lignans, where the stereochemistry of the benzylidene lactone is found to control the mode of cyclization. The *Z*-isomer undergoes mostly *6-endo*-cyclization and provides the desired (-)-isopodophyllotoxin along with a minor amount of *5-exo*-cyclized product, but the *E*-isomer goes through exclusively *5-exo*-cyclization leading to the undesired dihydroindenolactone compound instead of (-)-podophyllotoxin. The experimental results are well supported by the DFT studies.

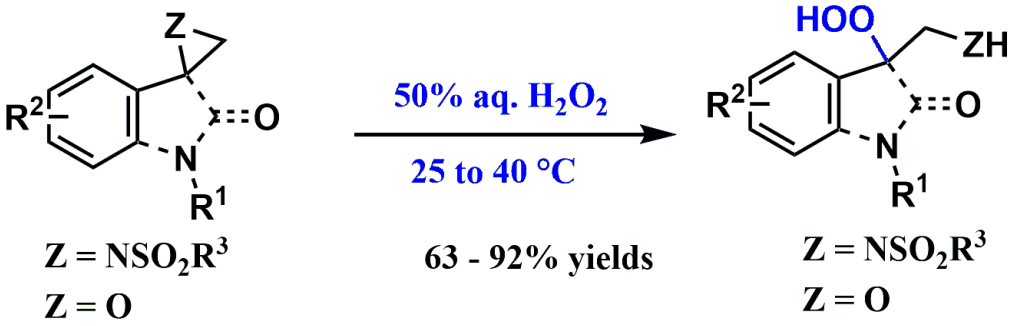


Regioselective Hydroperoxylation of Aziridines and Epoxides Only with Aqueous Hydrogen Peroxide

SK Abu Saleh, Atanu Hazra, Saumen Hajra (2022). ***Advanced Synthesis & Catalysis***, 364 (2): 391-404.

Organic hydroperoxides are prevalent unit in various natural products and bioactive compounds.These are also used as the synthetic precursor of therapeutically valuable endoperoxides. Additionally, benzylic hydroperoxides are extensively used as the antecedents for oxygen-centered radicals in polymer science, bioorganic and organometallic chemistry. Thus, the incorporation of hydroperoxide moiety into organic frameworks is highly demanding. In recent times, several methods have been developed based on singlet oxygen reaction with alkenes and alkanes, but most of them suffer from the narrow substrate scope. Again, the use of adverse peroxidation reaction conditions are not ideal from the environmental point of view. Aqueous hydrogen peroxide (H_2O_2),an operationally simple and commercially available reagent, is a superior source of hydroperoxide (-OOH) unit. Despite its many advantages, there are only a few reports on direct hydroperoxylation by exploiting aq. H_2O_2.

Here a catalyst and organic solvent-free regioselective hydroperoxylation of aziridines and epoxides, including spiroaziridine- and spiroepoxy oxindoles have been explored with commercially available 50% aq. H_2O_2. This method provides easy and direct access to secondary benzylic β-hydroperoxy amines and -alcohols and tertiary 3-hydroperoxy oxindoles. The protocol has also been applicable to the less reactive alkyl aziridines. Furthermore, an acid-catalyzedKornblum-DeLaMare type rearrangement of secondary benzylic hydroperoxide has also been revealed to afford amino- and hydroxyl ketones.

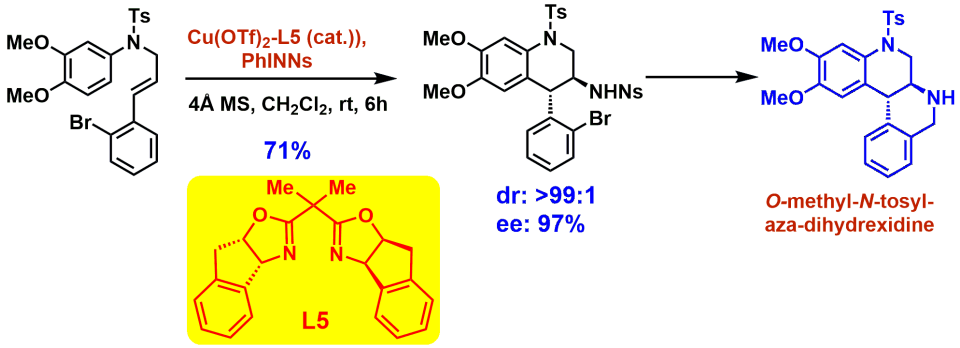


Asymmetric Aminoarylation for the Synthesis of *trans*-3-Amino-4-aryltetrahydroquinolines: An Access to Aza-Analogue of Dihydrexidine

SK Md. Samim Akhtar, Sukanta Bar and Saumen Hajra (2022). ***Tetrahedron***, 103: 132257.

Chiral 1, 2, 3, 4-tetrahydroquinolines, particularly, 3-aminotetrahydroquinolines and 4-aryltetrahydroquinolines feature in numerous pharmacological agents and natural products. Further, 3-amino-4-aryltetrahydroquinoline may emerge with dopaminergic property in the form of aza-analogue of dihydrexidine and doxanthrine, the two selective dopamine D1 agonists and potential drug candidates for the treatment of Parkinson's disease. Thus, extensive research efforts were made in the synthesis of substituted tetrahydro quinolines, but the asymmetric synthesis of 3-aminotetrahydroquinolines are still sparse in the literature.

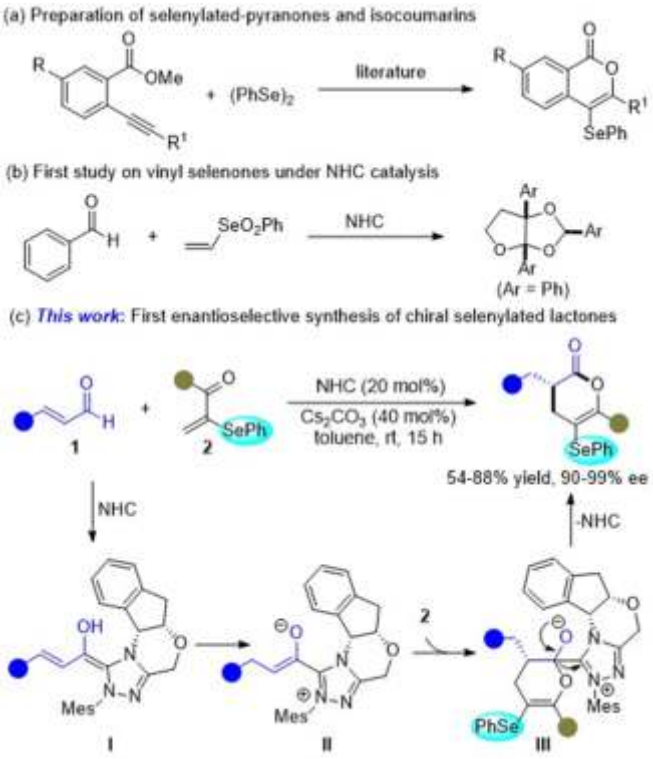
Here, a proficient stereoselective aminoarylation reaction of *N*-cinnamylanilines, based on atwo-step protocol of catalytic enantioselective aziridination and subsequent *6-endo-tet* Friedel-Crafts cyclization, has been developed and demonstrated. A pair of chiral bis-oxazoline ligand and $Cu(OTf)_2$offered an effective combination in the synthesis of *trans*-3-amino-4-aryltetrahydroquinolines with excellent diastereo- and enantioselectivity (dr: >99: 1 and ee up to 97%). In continuation, a *trans*-3-amino-4-aryltetrahydroquinoline, availed in one-pot stereoselective aminoarylation reaction, was extended toward a concise synthesis of aza-analogue of dihydrexdine, a potent and selective full dopamine-D1 agonist



Carbene Catalyzed Asymmetric Synthesis of Selenylated δ-Lactones via [4+2] Annulation of Selenyl Vinyl Ketones and Enals

Ram Subhawan Verma, Ranadeep Talukdar, Tazeen Azaz, Bhoopendra Tiwari (2022). ***Advanced Synthesis & Catalysis***, 364 (23): 4031-4035

The organoselenium compounds have attracted considerable attention because of their pharmacological value and natural occurrence in proteins and enzymes. They also act as antioxidants, help in maintaining intracellular redox status, production of thyroid hormone, etc. In addition, they are widely used as the versatile building blocks and catalysts in organic synthesis. Consequently, numerous methods have been developed for the preparation of organoselenium compounds. These methods generally produce achiral products. A very limited success has been achieved for the enantioselective synthesis. Functionalized dihydropyranones and their derivatives like pyranones and isocoumarins are the core structures of many pharmaceuticals like enzyme inhibitors, antibiotics, antifungal, antiviral, phytotoxic agents, agrochemicals, pheromones, etc. On the other hand, the functionalization of organic molecules with selenyl groups often augment their physical, chemical and biological properties. Thus, it is expected that selenylated dihydropyranones can have improved activity/properties compared to their parent molecules for several potential applications. Our literature search did not produce any direct method for the preparation of such chiral products. A direct (organo)catalytic method for the synthesis of chiral selenylated δ-lactones via [4+2] annulation of selenyl vinyl ketones with enals has been achieved. The C5-selenylated dihydropyranones were obtained The C5-selenylated dihydropyranones were obtained in 54-88% yield with 90–99% enantioselectivity.



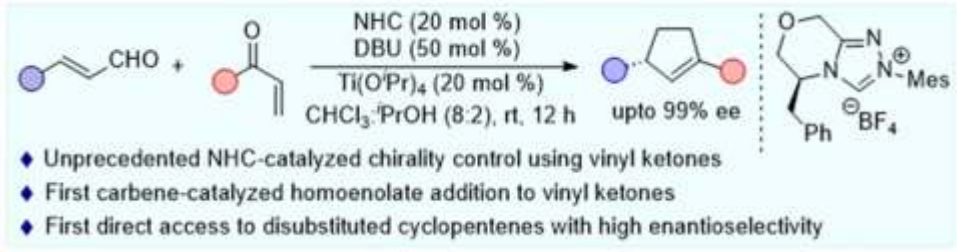
NHC-catalyzed enantioselective preparation of Selenylated δ-Lactones

N-Heterocyclic Carbene Catalyzed Enantioselective [3+2] Annulation of Enals with Vinyl Ketones

Tazeen Azaz, Hemlata Mourya, Vikram Singh, Bali Ram, Bhoopendra Tiwari (2022). ***The Journal of Organic Chemistry***, 88 (2): 1219–1226

Controlling the reaction pathways stereoselectively to afford the desired products for reactions having multiple potential reactivity is one of the primary goals in organic synthesis. *N*-Heterocyclic Carbene (NHC)-catalyzed reaction of enals with enones is one among them. Despite progress, the substitution at β-position on enones has remained critical for the reactivity as well as enantiocontrol. The literature methods have largely remained unviable for vinyl ketones (β-unsubstituted enones) probably due to lesser steric hindrance that plays an important role in stereocontrol as well in regioselectivity. To the best of our knowledge, an enantioselective synthesis from vinyl ketones *via* enolates, homoenolates or acyl anions is still elusive. Moreover, a carbene-catalyzed direct method for accessing disubstituted cyclopentenes has remained unknown yet.

An unprecedented carbene-catalyzed enantioselective [3+2] annulation of enals with vinyl ketones has been achieved. Unlike chalcones, the β-unsubstituted enones, vinyl ketones, have remained challenging in terms of reactivity, especially enantioselectivity. The disubstituted cyclopentenes were obtained in good yield and excellent stereoselectivity in the presence of $Ti(O^iPr)_4$.



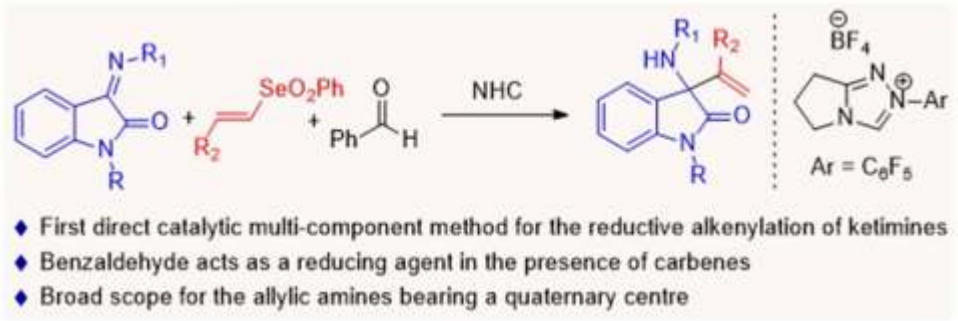
NHC-catalyzed enantioselective preparation of disubstituted cyclopentenes

Reductive Alkenylation of Ketimines via Hydride Transfer from Aldehydes

Tazeen Azaz, Hemlata Mourya, Vikram Singh, Bali Ram, Bhoopendra Tiwari (2022).
The Journal of Organic Chemistry, 88 (1): 632–639

Functionalized oxindoles bearing a α-tertiary amine center at C-3 position (a quaternary centre) represent an important class of heterocyclic framework in medicinal chemistry and natural products. These compounds exhibit an extensive range of pharmacological effects that include antiviral, antibacterial, antifungal, anticancer, anti-inflammatory and antihypertensive activities. Consequently, the development of novel routes for the synthesis of 3-amino oxindole-derived compounds has attracted considerable attention. A reductive functionalization of isatin-derived ketimines represents one such fundamental reaction for the direct access to these class of useful moieties.

The first direct *N*-Heterocyclic Carbene (NHC)-catalyzed preparation of allylic amines bearing a quaternary center (α-tertiary amine) from isatin-derived ketimines in the presence of vinyl selenones and aldehydes is reported. This multicomponent reaction is expected to proceed *via* unprecedented in-situ reduction of imines through a hydride transfer from the aldehydes.



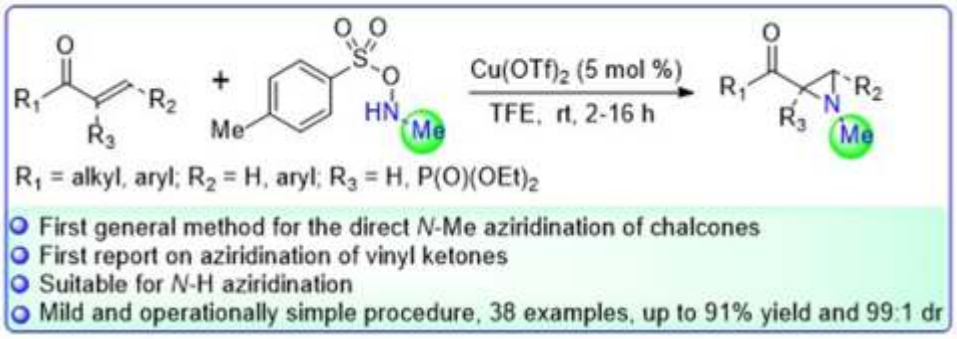
NHC-catalyzed reductive alkenylation of Isatins

Direct N-Me Aziridination of Enones

Jawahar L. Jat, Ajay K. Yadav, Chandra Bhan Pandey, Dinesh Chandra, Bhoopendra Tiwari (2022). ***The Journal of Organic Chemistry***, 87: 3751-3757

Aziridines are the attractive three-membered aza-heterocyclic scaffolds present in many bioactive molecules and natural products. They also behave as reactive intermediates in organic synthesis for accessing many nitrogen-containing products owing to their strained-ring system, enabling their facile participation in cycloaddition, carbonylative ring expansion and rearrangement reactions. Consequently, their preparation garnered a significant attention and the initial success was achieved mainly for the preparation of activated aziridines (e.g., *N*-Ts, *N*-Ns, *N*-acyl). The unactivated aziridines (e.g., *N*-H and *N*-Me) were accessed mainly through multi-step processes. In 2014, Falck and coworkers developed the first direct method for *N*-H and *N*-Me aziridination of electron-rich olefins, followed by Electron-deficient olefins like *α,β*-unsaturated-ketones, acids, amides are widely used substrates in organic synthesis, and their *N*-H and *N*-Me/alkyl aziridines are present in many bioactive natural products. Consequently, the development of efficient methods for the preparation of *N*-H and *N*-Me/alkyl aziridines is essential. In that direction, numerous reports dedicated to *N*-H aziridination of chalcones have appeared in the recent past. Our previous Rh(II) catalyzed method for the electron-rich olefins was not suitable for the electron-deficient chalcones and vinyl ketones. To the best of our knowledge, there is no precedence on the direct general method for *N*-Me aziridination of chalcones. Moreover, vinyl ketones, and the enones bearing a bulkier *α*-substitution have remained challenging for the known methods of aziridination (*N*-H as well as *N*-Me). Therefore, any method in that direction is highly novel and desired.

The first direct general method for *N*-Me aziridination of electron-deficient olefins, enones, is described using *N*-methyl-*O*-tosylhydroxylamine as the aminating agent in the presence of $Cu(OTf)_2$ catalyst. The aziridination of vinyl ketones, hitherto unknown for *N*-Me as well as *N*-H, has been achieved efficiently. The open-flask reaction is stereospecific, operationally simple and additive-free. It also affords *N*-H aziridinated products under a similar reaction condition efficiently.



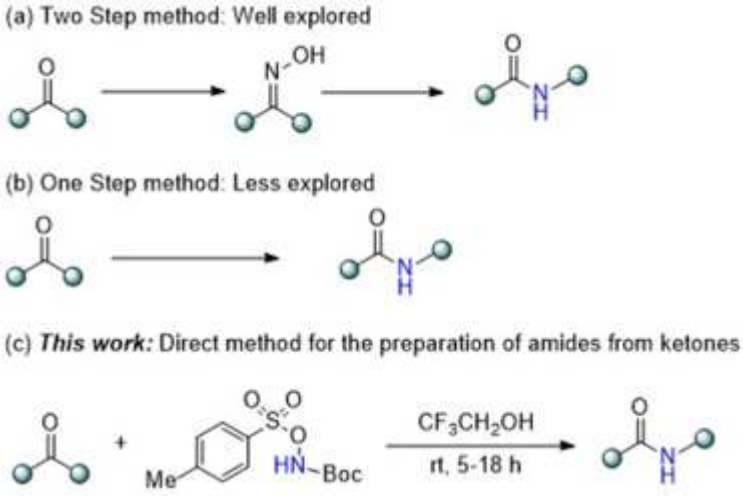
Direct aziridination of enones

Metal-free Synthesis of Secondary Amides Using N-Boc-O-Tosylhydroxylamine as Nitrogen Source via Beckmann Rearrangement

Jawahar Lal Jat , Puneet Kumar, Saumya Verma , Dinesh Chandra, Vikram Singh, Bhoopendra Tiwari
(2022). ***New Journal of Chemistry***, 46: 14782 – 14785

Secondary amides portray fascinating structural subunits in various important bioactive natural products and drug candidates as well as in polymers, dyes, textiles, and agrochemical products. They also form versatile synthetic intermediates for the preparation of a diverse range of alkaloids, and nitrogen and oxygen containing valuable compounds. Additionally, the *sec*-amides have emerged as a preferred directing group for a selective C-H bond activation. As a result, the amide bond synthesis is one of the most frequently used synthetic reactions.The trivial method for their preparation through coupling of carboxylic acids and amines have several intrinsic limitations. For example, a requirement of an expensive (and often stoichiometric) reagent for the activation of carboxylic acid, generation of toxic waste and poor atom economy that limit their wide applications in industries.

Ketones are widely available and stable synthones, and therefore, they have been explored for the amide synthesis for a long time. The discovery of Beckmann rearrangement (BKR) was a milestone in this direction, transforming the preformed ketoximes to amides in an acidic media. This approach successfully eliminated the major drawbacks associated with the methods relying on the use of carboxylic acids as the substrates. Nonetheless, this two-step process starting from ketones generally requires a harsh reaction condition (strong acid and high temperature), rendering this procedure incompatible for sensitive substrates. Several improved studies have been reported recently for the Beckman rearrangements under milder conditions. Despite this notable progress, these methods have one or the other limitations like toxicity of reagents, high reaction temperature, limited substrate scopes, survival of sensitive functional and protecting groups, requirement of additives, tedious reaction/purification procedures, etc.



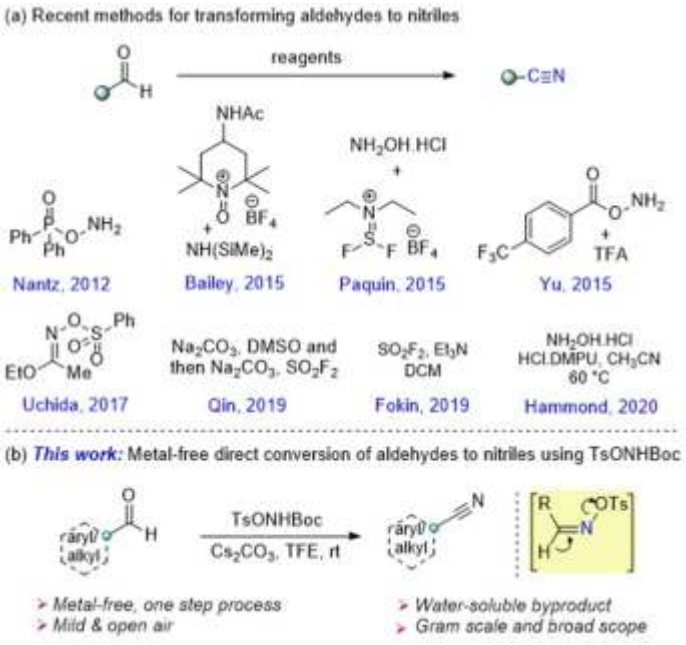
Metal-free synthesis of secondary amides

Herein, we report the first direct method for the synthesis of secondary amides from ketones *via* Beckmann rearrangement using *N*-Boc-*O*-tosylhydroxylamine (TsONHBoc) as the aminating agent. This reagent is expected to play a dual role, first in the formation of activated oxime intermediate, followed by facilitation of the amide formation as a Bronsted acid by the by-product, tosic acid. The metal and additive-free one-step method progresses in TFE solvent through *in situ* generation of primary amine reagent ($TsONH_2$), and produces a water-soluble by-product.

Metal-free Synthesis of Nitriles from Aldehydes Using N-Boc-O-Tosylhydroxylamine as Nitrogen Source

Puneet Kumar, Vikram Singh, Jawahar L. Jat, Bhoopendra Tiwari
(2022). ***New Journal of Chemistry***, 47 (2): 535 – 538.

The nitrile group is widely present in numerous bioactive natural products, drug candidates, agrochemicals, dyes and polymers. The presence of this functionality on many marketed drugs like escitalopram (for depression and anxiety), bicalutamide (for prostate cancer), milrinone (for heart failure), fadrozole (for breast cancer), rilpivirine (for AIDS) and nilvadipine (for hypertension) further highlights the significance of this class of molecules. Moreover, they find extensive applications in the preparation of amines, amides, esters, acids, aldehydes and heterocyclic compounds. The traditional methods for the preparation of nitriles are the Sandmeyer reaction, Rosenmund-von Braun reaction, halide-cyanide exchange reactions and cross-metathesis. These methods demand stoichiometric amounts of toxic metal cyanides. The cyanide-free alternatives *via* dehydration of amides or aldoximes require harsh reaction conditions and tedious procedure. A readily available low-cost aldehydes have emerged as an attractive substrate for the synthesis of nitriles. The Schmidt reaction provides a direct access to nitriles from aldehydes in the presence of azides (e.g., HN_3 or NaN_3/acid) under demanding reaction condition. A number of improved methods have been reported using a variety of nitrogen source. Despite this progress, the toxicity, stability and accessibility of the reagents, harsh reaction condition, functional group tolerance, cost, etc. have remained yet to be fully resolved. Therefore, development of newer methods for the preparation of nitriles continues to be of great significance and highly desirable.



Transition metal-free synthesis of secondary amides

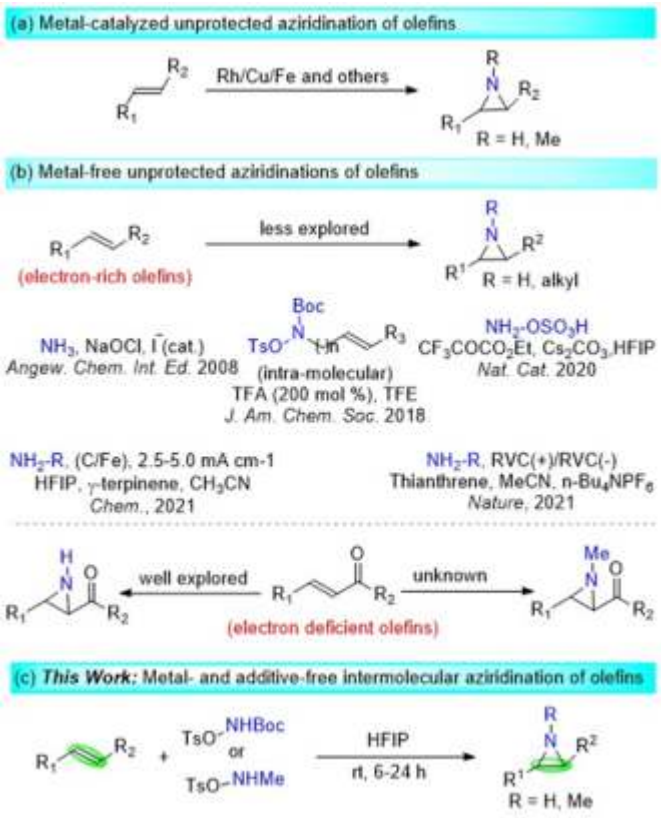
Herein, we have demonstrated an economical and practical approach to nitriles from readily available aldehydes using stable *N*-Boc-*O*-tosylhydroxylamine (TsONHBoc) as the aminating agent. This direct transition metal-free method tolerates a wide range of functional groups and provides aromatic, aliphatic, allylic, heteroarylic and α,β-unsaturated nitriles in excellent yields. Bench-stability, ease of handling and *in situ* generation of highly reactive *N*-source under a mild and benign reaction condition add additional advantages for a potential scale-up synthesis.

Metal and Additive-Free Intermolecular Aziridination of Olefins Using N-Boc-O-Tosylhydroxylamine

Jawahar L. Jat, Dinesh Chandra, Puneet Kumar, Vikram Singh, Bhoopendra Tiwari (2022).
Synthesis, 54(20): 4513 – 4520.

The development of improved synthetic methods for the preparation of the smallest saturated azaheterocycles, aziridines, has attracted significant attention in the recent past. They not only form important building blocks but also exist as substructures in many bioactive molecules. For example, aziridines serve as a crucial precursor for many drugs such as ()-oseltamivir, ()-lycoricidine, ()-agelastatin A, etc. Traditionally, they were obtained in a protected/activated form (e. g., *N*-Ts, *N*-Ns, *N*-acyl) through the cyclization of amino- or azido-alcohols, addition of carbenes to imines or transfer of nitrenes to olefinic bonds. The direct synthesis of non-activated aziridines (*N*-H, *N*-alkyl) from alkenes remained challenging till recent. Initially, the success in this direction was achieved on unactivated olefins using Rh catalyst and hydroxyl amine derived 2,4-dinitrophenyl hydroxylamine (DPH), hydroxylamine-O-sulfonic acid (HOSA) or *O*-(mesitylsulfonyl)hydroxylamine (MSH) as one of the aminating reagents, reported by the groups of Falck, Kurti, and Jat and Tiwari.

Accessing useful scaffolds under a transition metal-free condition offers several unique advantages and therefore remains one of the top priorities in organic synthesis. Despite magnificent development, the literature methods in general have one or the other limitations such as the requirement of expensive metal catalysts, additives, explosive or toxic reagents, limited substrates scope, interference of byproduct, etc. Our literature search did not produce any report on the aziridination of unactivated alkenes that excludes the use of both the metal catalysts as well as additives and hence any such method is highly desirable. Herein we report an unprecedented metal and additive-free direct atom-economical method for the aziridination of unactivated alkenes using *N*-Boc-*O*-tosylhydroxylamine (TsONHBoc) in hexafluoro-isopropanol (HFIP) solvent. The use of TsONHBoc that *in situ* generates the free aminating agent under the reaction condition inherits several advantages over the other similar agents, such as low cost, easy access and stability (non-explosiveness) during the storage over a longer time.

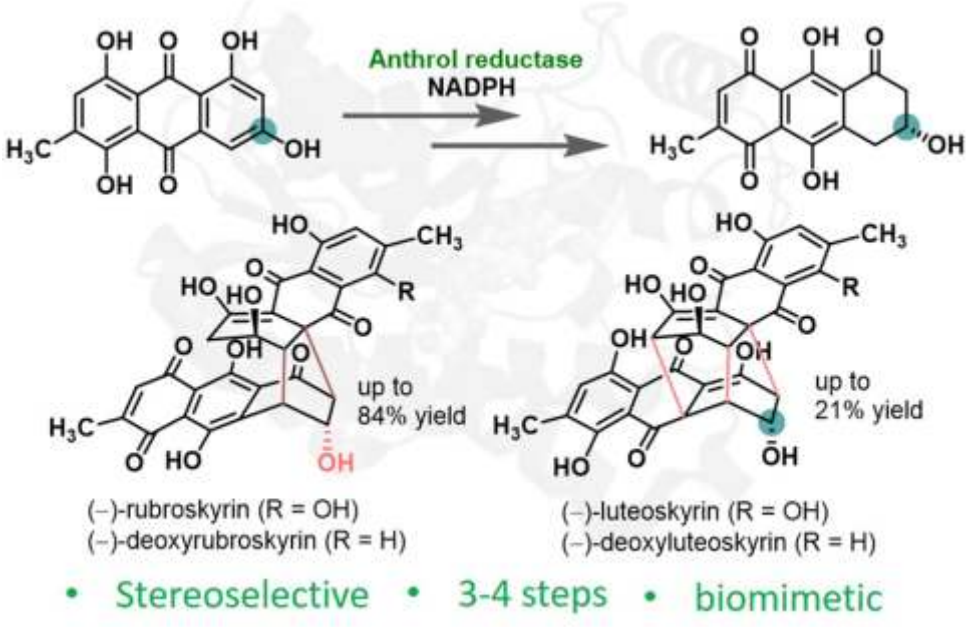


Direct N-H and N-Alkyl Aziridination of Olefins

Concise chemoenzymatic total synthesis of (−)-rubroskyrin, (−)-deoxyrubroskyrin (−)-luteoskyrin, and (−)-deoxyluteoskyrin

Amit Mondal, Nirmal Saha, Syed Masood Husain (2022). ***Tetrahedron Chem***, 3: 100030.

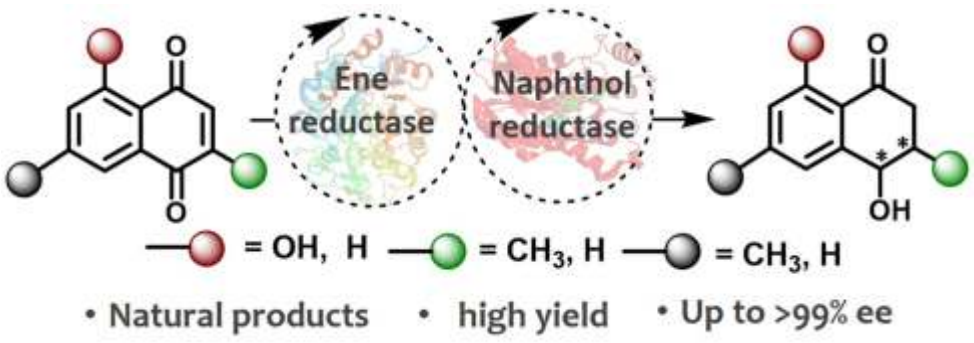
Synthesis of complex dimeric natural products (−)-luteoskyrin and (−)-deoxyluteoskyrin isolated from *P. islandicum* Sopp nearly 70 years ago, remained a challenge until now. Their biosynthesis had been proposed to involve dimerization using a putative intermediate dihydrocatenarin as a key step. In the current work, we employed a chemoenzymatic strategy to synthesize (*R*)-dihydrocatenarin using an anthrol reductase of *T. islandicus*. Its homodimerization in the presence of molecular oxygen gave (−)-rubroskyrin, which on Michael reaction led to the first total synthesis of (−)-luteoskyrin in an overall yield of 21%. In contrast, the heterodimerization between (*R*)-dihydrocatenarin and (*R*)-dihydroemodin led to non-natural, (−)-deoxyrubroskyrin analogue, while the use of molecular oxygen gave natural (−)-deoxyrubroskyrin. Both (−)-deoxyrubroskyrin and its analogue on treatment with pyridine gave (−)-deoxyluteoskyrin with an overall yield of up to 10%. The presence of dihydrocatenarin in *P. islandicum* NRRL 1036 culture is verified through mass spectrometry, which implied a similar biosynthetic pathway.



Highly efficient one-pot multienzyme cascades for the stereoselective synthesis of natural naphthalenones

Arijit De, Nirmal Saha, Tanaya Manna, Vidya Singh, Syed Masood Husain (2022). ***ACS Catalysis***, 12 (19): 12179 – 12185.

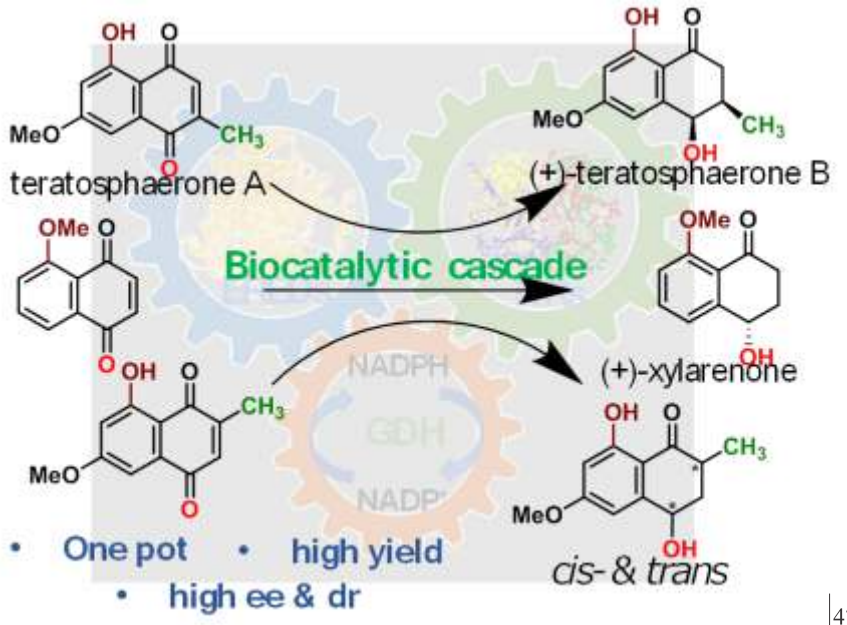
Naphthaleneones are a class of polyketidic natural products widely distributed in plants and fungal species. Among these, the 3-methyl substituted naphthalenones such as *cis*-isoshinanolones, *trans*-isoshinanolone and its biosynthetic precursor, plumbagin were isolated first from a plant, *Diospyros maritima*by Tezuka. Since, then all the stereoisomers of isoshinanolones have been reportedly isolated from several plant species that includes *Dioncophyllumthollonii*, *Habropetalum Dawei*, *Plumbago scandens*, *Plumbago zeylanica*, and *Ancistrocladus heyneanus*, and *Ancistrocladaceae* species endemic to India. In the current work, a biocatalytic cascade containing an ene-reductase (NostocER) and naphthol reductase (tetrahydroxynaphthalene or trihydroxynaphthalene reductase) of *Magnaporthe grisea* and NADPH is developed. The optimized multienzyme cascade is applied for the one-pot reduction of plumbagin to obtain biologically active *cis*-(3*R*,4*R*)-isoshinanolone, with dr *cis.rans* 98:2 and >99% ee in 96% yield. Furthermore, naturally occurring (+)-isosclerone, (+)-shinanolone, (−)-shinanolone, and (*S*)-4-hydroxy-3,4-dihydronaphthalen-1(2*H*)-one were also synthesized with excellent stereoselectivity and high yields (71–89%) using the enzymatic cascades. The investigation of NostocER–T_4HNR-cascade reduction of menadione, plumbagin, and 5-methoxymenadione revealed specificity of tetrahydroxynaphthalene reductase toward these substrates. In addition, the kinetic studies showed a high catalytic efficiency of NostocER and T_4HNR toward plumbagin and dihydroplumbagin, respectively, compared to other enzymes.



Asymmetric synthesis of (+)-teratosphaerone B, its non-natural analogue and (+)-xylarenone using an ene- and naphthol reductase cascade

Tanaya Manna, Arijit De, Khondekar Nurjamal, Syed Masood Husain (2022). ***Organic and Biomolecular Chemistry***, 20 (37): 7410 – 7414.

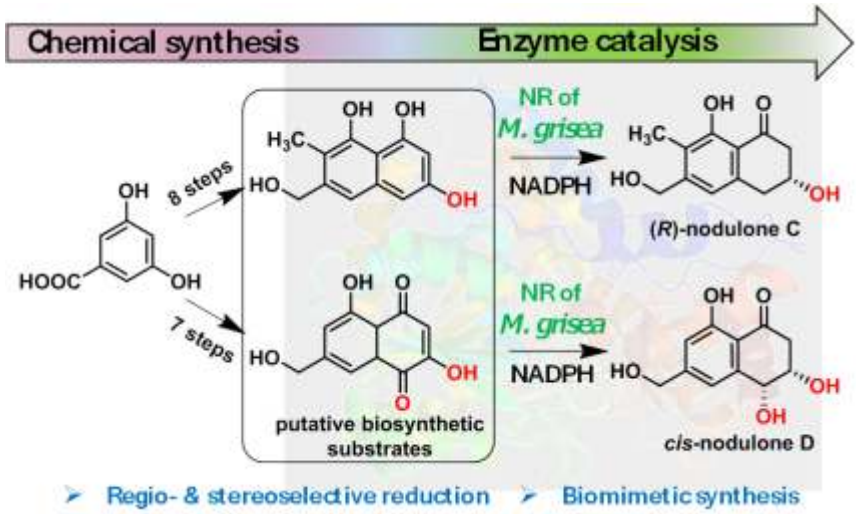
In recent years, the use of enzymatic cascades has emerged as a powerful tool for the effective synthesis of chiral building blocks, complex natural products, and pharmaceutically active drug molecules. Such cascades are often inspired by the biosynthetic pathways of natural products which uses multiple enzymes to catalyze various steps. Moreover, the use of enzymes offers an advantage over tradition synthetic methods as it gives excellent chemo-, regio- and stereoselectivity along with high yields under mild reaction conditions. In the current work, we aim to develop a multienzyme cascade for the synthesis of natural naphthalenones, teratosphaerone B and xylarenone. The polyketidic natural products, teratosphaerone A and teratosphaerone B have been isolated recently from endophytic fungi *Teratosphaeria* sp. FL2137 associated with dead but undecomposed leaves of *Pinus clausa* (Pinaceae). To get access to these natural products using a multienzyme cascade, a one-pot bienzymatic cascade containing an ene and a naphthol reductase is developed. It is applied for the synthesis of (+)-(3*R*,4*R*)-teratosphaerone B, its non-natural regioisomer in both *cis*- and *trans*-forms and (+)-xylarenone by the reduction of chemically synthesized naphthoquinone precursors in high yields (76–92%) and excellent ee (>99%). This work implies similar biosynthetic steps in the formation of the synthesized natural products.



Chemoenzymatic total synthesis of nodulones C and D using a naphthol reductase of *Magnaporthe grisea*

Tanaya Manna, Arijit De, Khondekar Nurjamal, Syed Masood Husain (2022). ***Organic and Biomolecular Chemistry***, 20 (37): 7410 – 7414.

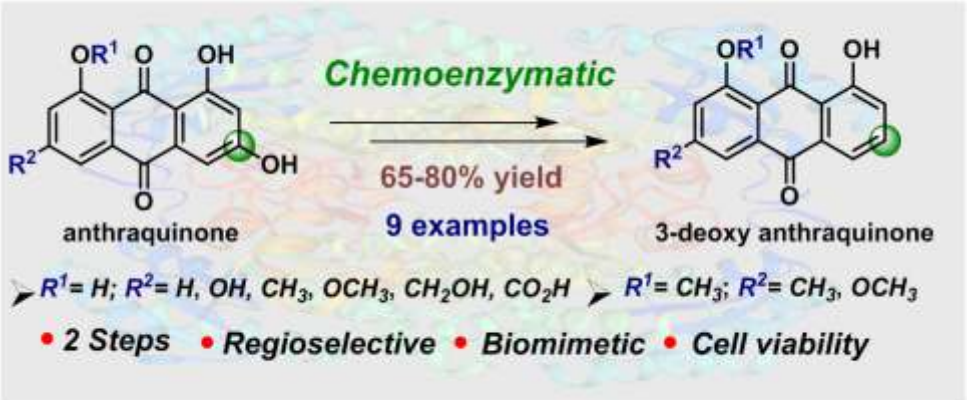
Endophytic fungi are known to produce a large number of secondary metabolites with diverse structural features, which display a wide array of biological activities. Among these, nodulones A-E belong to a new class of bioactive polyketides produced by *Nodulisporium sp.,* a group of common endophytic fungi harbored by many plants. Although the biosynthesis of nodulones A, B, C and D isolated from *D. eschscholtzii* has been proposed, little is known about the enzymes involved in their formation. Furthermore, despite their fascinating architecture and useful biological activities, no synthesis is reported for the preparation of chiral nodulones thus far. We speculated the involvement of naphthol reductase like enzymes in the biosynthesis of nodulones. Therefore, a blast was performed to search for the T_4HNR and T_3HNR of *M. grisea* related genes. We found that T_3HNR like gene (AFO12495.1) was indeed present in the genome of *D. eschscholtzii* (taxid: 292717), which is known to produce a variety of nodulonesand shows 82% sequence identity. This led us to hypothesize that T_4HNR or T_3HNR can be used in a chemoenzymatic synthesis of chiral nodulones A-D. In the current work, the asymmetric and chemoenzymatic synthesis of (*R*)-nodulone C, *cis*-nodulone D and related (*R*)-dihydronaphthalenone is reported. It involves multistep chemical synthesis of putative biosynthetic substrates followed by regio- and stereoselective reduction using a NADPH-dependent tetrahydroxynaphthalene reductase of *Magnaporthe grisea* to obtain chiral nodulones in a biomimetic fashion.



A biocatalytic approach towards the preparation of natural deoxyanthraquinones and their impact on cellular viability

Anshul Rajput, Arijit De, Amit Mondal, Kiran Das, Biswanath Maity, Syed Masood Husain (2022). ***New Journal of Chemistry***, 46: 3087 – 3090.

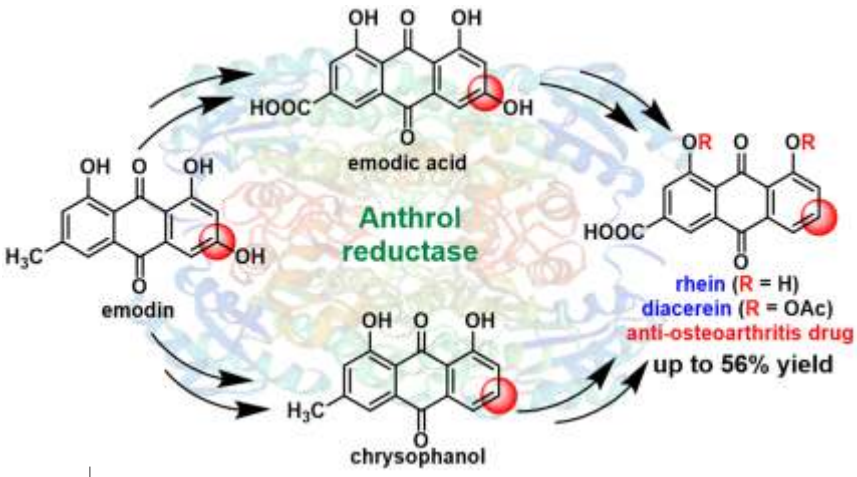
Anthraquinones is a large group of aromatic polyketides, with approximately 700 compounds isolated from plants, lichens and fungi. Besides their use as dyes, anthraquinones have been applied for medicinal purposes for centuries. Among these 3-deoxygenated anthra-9,10-quinones such as chrysophanol, aloe-emodin, 3-methoxychrysazin, rhein, 1,3,8-trihydroxy emodin, dantron and 1-O-methyl chrysophanol have a wide occurrence. These compounds show a diverse array of biological activities which includes laxative, anticancer, antiarthritic, anti-inflammatory, antibacterial, antifungal, antiviral, antihyperglycemic and neurodegenerative effects. The biosynthesis of anthraquinones in fungi usually involves the condensation of monomeric acetyl-CoA and malonyl-CoA to octaketide by the polyketide synthase (PKS), which on regioselective cyclization and aromatization forms anthraquinones. These anthraquinones on modification by the cluster of enzymes form various deoxygenated anthraquinones. In the current work, a two-step chemoenzymatic process for the synthesis of medicinally important 3-deoxygenated anthra-9,10-quinones is developed. It involves a regio- and stereoselective reduction of hydroanthraquinones to (*R*)-configured dihydroanthracenones using an anthrol reductase of *T. islandicus*, followed by oxidation and dehydration to obtain deoxyanthraquinones in 65–80% yield. Comparison of the cell viability of normal human kidney HEK293 cells between anthraquinones and their deoxy derivatives revealed less toxicity for the latter.



Synthesis of rhein and diacerein: a chemoenzymatic approach using anthrol reductase of *Talaromyces islandicus*

Anshul Rajput, Amit Mondal, Satyendra Kumar Pandey, Syed Masood Husain (2022). ***Organic & Biomolecular Chemistry***, 20: 358 – 361.

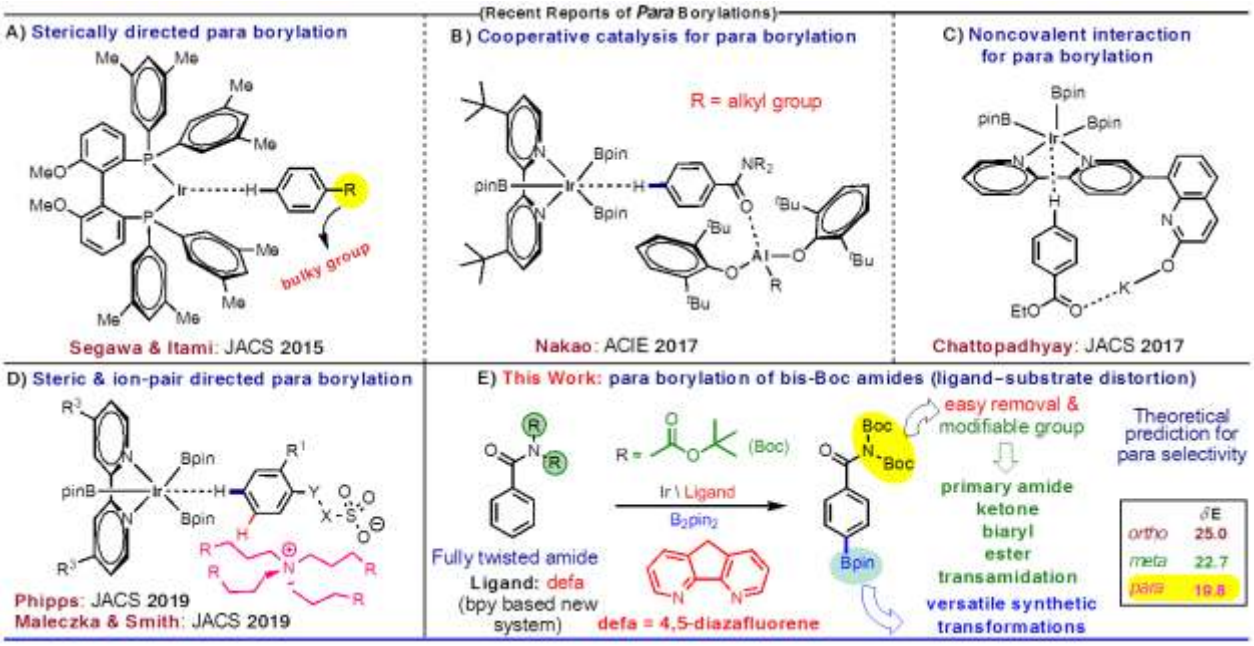
Arthritis is a general term for joint disorder featuring inflammation. Osteoarthritis (OA), the most common form of arthritis, is a chronic, degenerative disorder characterized by progressive destruction and erosion of articular cartilage. It affects millions of people worldwide and according to the World Health organisation (WHO), 10% of the world's population aged 60 or older have pain or disability from OA. For its treatment, diacerein, a diacetyl derivative of rhein is used as a symptomatic, slow-acting drug. Rhein being the actual metabolite of diacerein, that inhibits interleukin-1 activity with the aid of lowering the collagenase production in articular cartilage. Over the past few decades, several methods for the synthesis of anthraquinones have been developed which relies on Diels-Alder reactions, tandem approaches, organometallic reagents. Fries rearrangement, directed ortho metalation approach and the use of acid molten chloroaluminate. However, no biocatalytic approach is being applied so far for the synthesis of rhein and diacerein. In the current work, we have described two short, chemoenzymatic methods for the total synthesis of rhein and diacerein involving highly stereo- and regioselective enzymatic reduction of emodic acid and emodin using anthrol reductase of *T. islandicus* (ARti-2). The method which involves reductive deoxygenation of emodic acid gives rhein in 54% yield in 5 steps. While the second approach which utilizes chrysophanol obtained via chemoenzymatic reduction of emodin gives diacerein in just 4 steps with an overall yield of 56%. By far these are the first chemoenzymatic synthesis of diacerein and may be used as an alternate to non-enzymatic synthesis. Our biomimetic chemoenzymatic approach for the conversion of emodic acid to rhein also implies a similar biosynthetic pathway in fungus for these metabolites with the involvement of NADPH dependent anthrol reductase like enzymes.



Iridium-Catalyzed Ligand-Controlled Remote para-Selective C–H Activation and Borylation of Twisted Aromatic Amides

Md Emdadul Hoque, Ranjana Bisht , Anju Unnikrishnan, Sayan Dey , Mirja Md Mahamudul Hassan, Saikat Guria, Rama Nand Rai, Raghavan B Sunoj, Buddhadeb Chattopadhyay
(2022).***Angewandte Chemie International Edition***, 61 (27):e202203539.

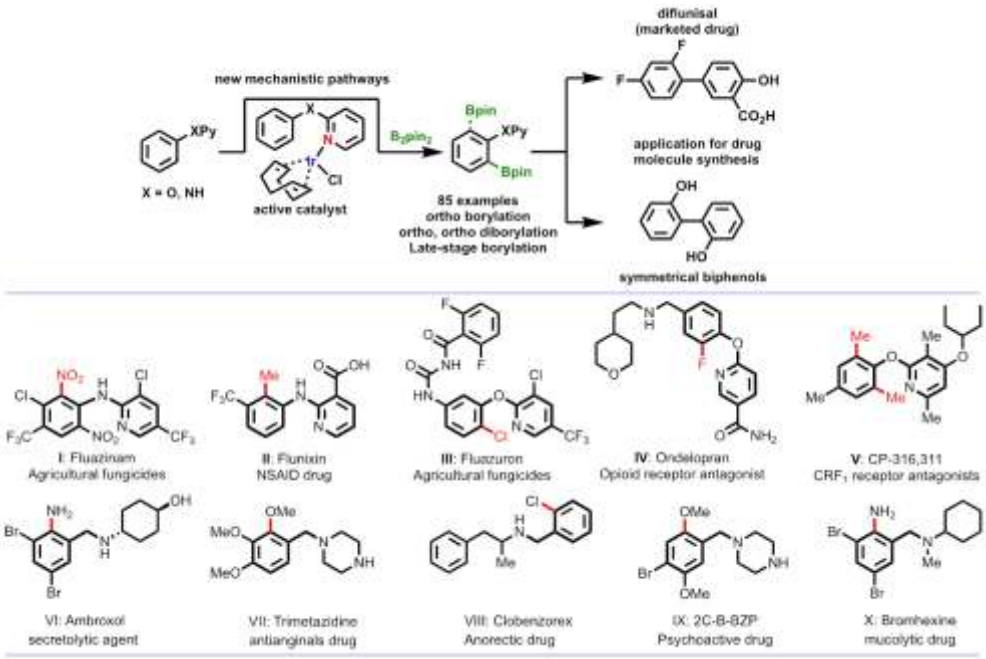
A method of para selective borylation of aromatic amides is described. The borylation proceeded via an unprecedented substrate–ligand distortion between the twisted aromatic amides and a newly designed ligand framework (defa) that is different from the traditionally used ligand (dtbpy) for the C–H borylation reactions. The designed ligand framework (defa) has led to the development of a new type of catalytic system that shows excellent para selectivity for a range of aromatic amides. Moreover, the designed ligand has shown excellent reactivity and selectivity for a range of heterocyclic aromatic amides. The identification of key transition states and intermediates using the DFT computations associated with the three regio-isomeric pathways revealed that the most efficient catalytic pathway with the defa ligand leads to the para borylation while in the case of bpy the borylation at the para and meta sites compete.



Ir-Catalyzed Ligand Free Directed C–H Borylation of Arenes and Pharmaceuticals: Detailed Mechanistic Understanding

Mirja Md Mahamudul Hassan, Biplab Mondal, Sukriti Singh, Chabush Haldar, Jagriti Chaturvedi, Ranjana Bisht, Raghavan B Sunoj, Buddhadeb Chattopadhyay (2022).
The Journal of Organic Chemistry, 87: 4360–4375.

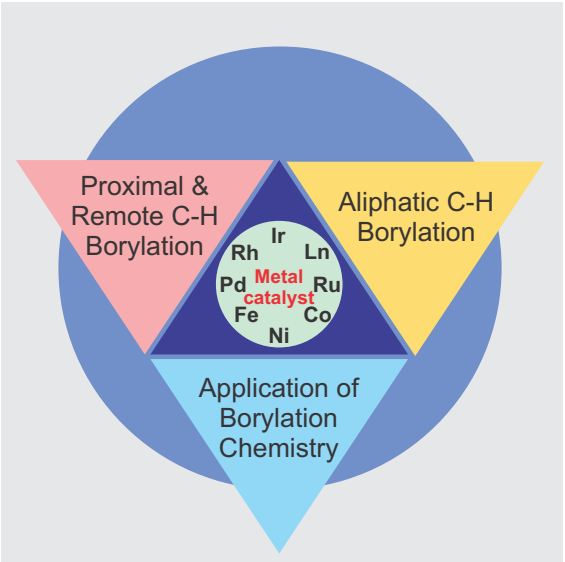
An efficient method for Ir-catalyzed ligand free ortho borylation of arenes (such as, 2-phenoxypyridines, 2-anilinopyridines, benzylamines, benzylpiperazines, benzylmorpholines, benzylpyrrolidine, benzylpiperidines, benzylazepanes, -amino acid derivatives, aminophenylethane derivatives, and other important scaffolds) and pharmaceuticals has been developed. The reaction underwent via an interesting mechanistic pathway, as revealed by the detailed mechanistic investigations by using kinetic isotope studies and DFT calculations. The catalytic cycle is found to involve the intermediacy of Ir-boryl complex where the substrate C-H activation is the turn-over determining step, intriguingly without any appreciable primary KIE. The method displays a broad range of substrate scope and functional group tolerance. Numerous late-stage borylation of various important molecules and drugs were achieved using this developed strategy. The borylated compounds were further converted into more valuable functionalities. Moreover, utilizing the benefit of the B–N intramolecular interaction of the mono borylated compounds, an operationally simple method has been developed for the selective diborylation of 2-phenoxypyridines and numerous functionalized arenes. Furthermore, the synthetic utility has been showcased with the removal of the pyridyl directing group from the borylated product to achieve ortho borylated phenol along with the ipso-borylation for the preparation of 1,2-diborylated benzene.



Metal-Catalysed C-H Bond Activation and Borylation

Ranjana Bisht, Chabush Haldar, Mirja Md Mahamudul Hassan, Md Emdadul Hoque, Jagriti Chaturvedi, Buddhadeb Chattopadhyay (2022). ***Chemical Society Reviews***, 51 (12): 5042-5100.

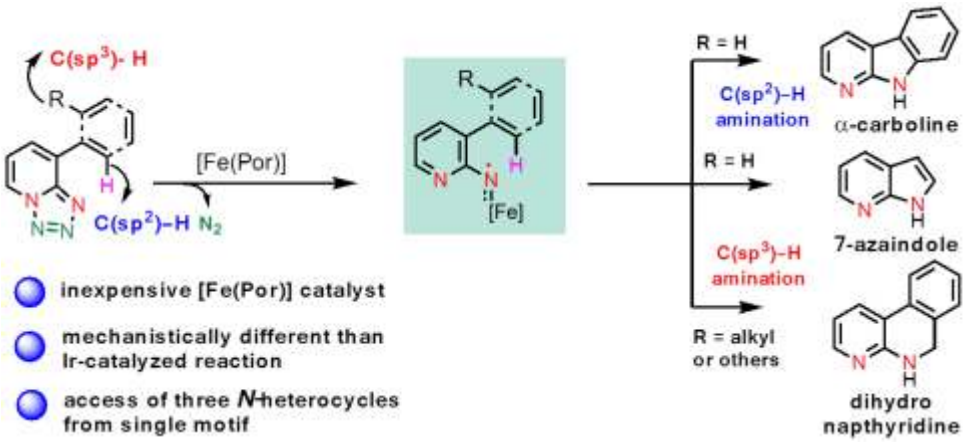
Transition metal-catalysed direct borylation of hydrocarbons via C–H bond activation has received a remarkable level of attention as a popular reaction in synthesis owing to the synthetic versatility of the organoboron compounds. While controlling the site-selectivity was one of the most challenging issues in these C–H borylation reactions, enormous efforts of several research groups proved instrumental in dealing with selectivity issues that presently reached an impressive level for both the proximal and distal C-H bond borylation. For example, in the case of ortho C–H bond borylation reactions, innovative methodologies have been developed based on either the modification of the directing groups attached with the substrates or by creating new catalytic systems via the design of new ligand frameworks. Whereas meta and para selective C-H borylations remained a formidable challenge, numerous innovative concepts have been developed within a very short period of time by the development of new catalytic systems with the employment of various noncovalent interactions. Moreover, significant advancements have occurred for the aliphatic C(sp^3)-H borylations as well as enantioselective borylations. In this review article, we aim to discuss and summarize the different approaches and findings related to the development of the directed proximal ortho, distal meta/para, aliphatic (racemic and enantioselective) borylation reactions since 2014. Additionally, considering the C–H borylation reaction as one of the most important mainstream reactions, various applications of this C-H borylation reaction toward the synthesis of natural products, therapeutics, and applications in materials chemistry will be summarized in the last part of this review article.



An Iron (II)-Based Metalloradical System for Intramolecular Amination of C(sp²)-H and C(sp³)-H Bonds: Synthetic Applications and Mechanistic Studies

Sandip Kumar Das, Subrata Das, Supratim Ghosh, Satyajit Roy, Monika Pareek, Brindaban Roy, Raghavan B. Sunoj, Buddhadeb Chattopadhyay (2022). ***Chemical Science***, 13: 11817-11828.

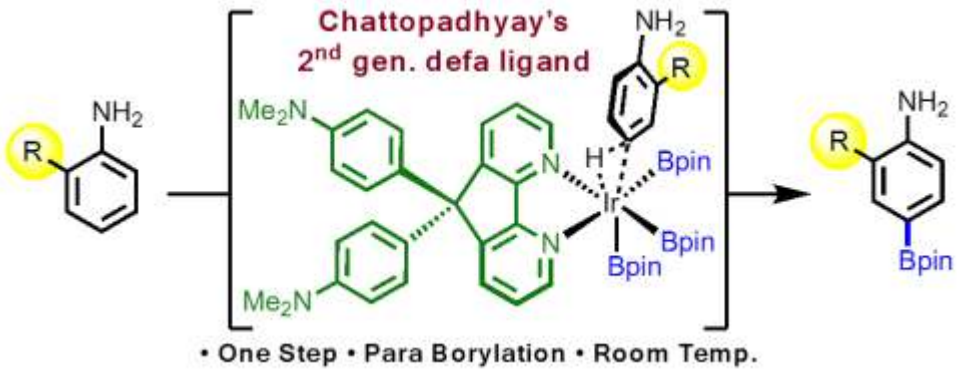
A catalytic system for intramolecular C(sp²)-H and C(sp³)-H amination of substituted tetrazolopyridines has been successfully developed. The amination reactions are developed using an iron-porphyrin based catalytic system. It has been demonstrated that the same iron-porphyrin based catalytic system efficiently activate both the C(sp²)-H and C(sp³)-H bonds of the tetrazole as well as azide-featured substrates with high level of regioselectivity. The method exhibited excellent functional group tolerance. The method affords three different classes of high-valued N-heterocyclic scaffolds. A number of important late-stage C-H aminations have been performed to access important classes of molecules. Detailed studies (experimental and computational) showed that the both the C(sp²)-H and C(sp³)-H amination reactions involve a metal oradical activation mechanism, which is different from the previously reported electro-cyclization mechanism. Collectively, this study reports the discovery of new class of metalloradical activation mode using base metal catalyst that should find wide application in the context of medicinal chemistry, drug discovery and industrial application.



Ligand and Substrate-Controlled Para C-H Borylation of Anilines at Room Temperature

Chabush Haldar, Ranjana Bisht, Jagriti Chaturvedi, Saikat Guria, Mirja Md Mahamudul Hassan, Bali Ram, Buddhadeb Chattopadhyay (2022). ***Organic Letters***, 24 (44): 8147–8152.

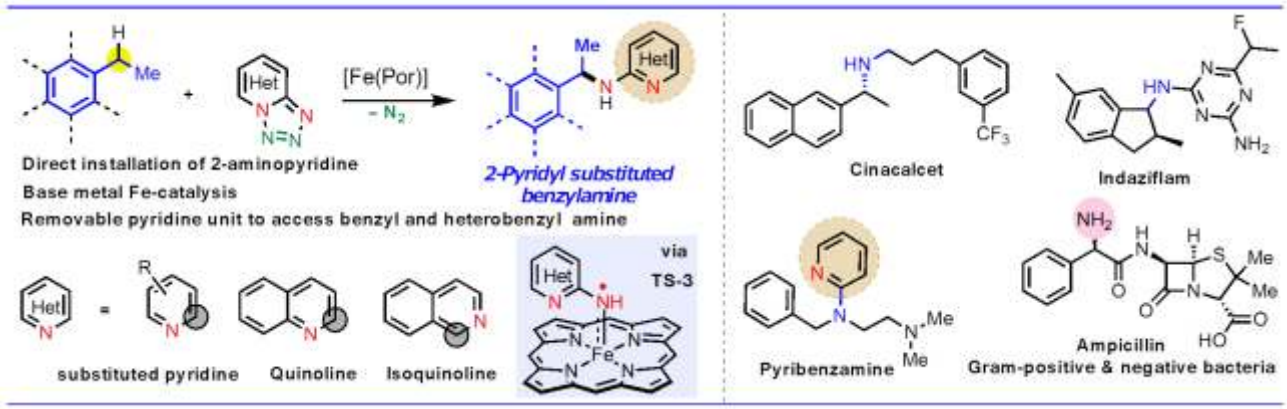
A new catalytic method for para borylation of unprotected anilines is described. The catalytic method is developed by designing a new type of ligand framework that enables the para borylation at room-temperature. We showed that whereas previously reported para borylation of 2-substituted anilines required multi-step protection/deprotection sequences and high reaction temperature, our method give a straightforward solution for achieving para borylation without such protection/deprotection chemistry at room-temperature.



Iron-Catalyzed Intermolecular Amination of Benzylic C(sp^3)–H Bonds

Hillol Khatua, Subrata Das, Sima Patra, Sandip Kumar Das, Satyajit Roy, Buddhadeb Chattopadhyay (2022). ***Journal of the American Chemical Society***, 144 (48): 21858-21866.

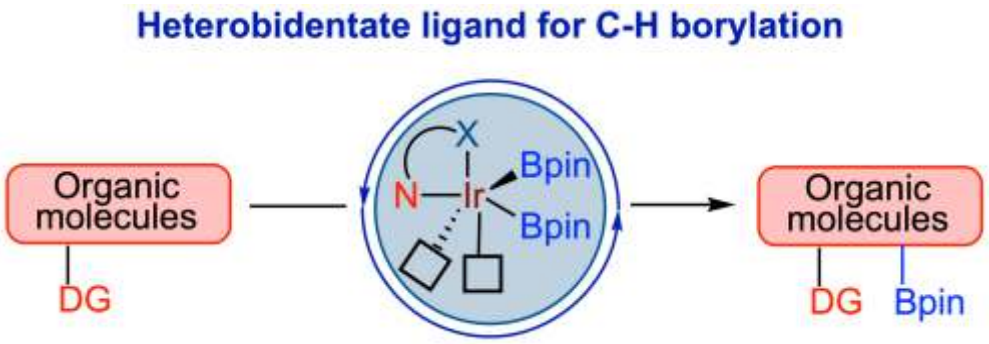
A catalytic system for intermolecular benzylic C(sp^3)–H amination is developed utilizing 1,2,3,4-tetrazole as a nitrene precursor via iron catalysis. This method enables direct installation of 2-aminopyridine into the benzylic and heterobenzylic position. The method selectively aminates 2^o benzylic C(sp^3)–H bond over the 3^o and 1^o benzylic C(sp^3)–H bonds. Experimental studies reveal that the C(sp^3)–H amination undergoes via the formation of a benzylic radical intermediate. This study reports the discovery of new method for 2-pyridine substituted benzylamine synthesis using inexpensive, biocompatible base metal catalysis that should find wide application in the context of medicinal chemistry and drug discovery.



Catalyst Engineering through Heterobidentate (N-X type) Ligand Design for Iridium-Catalyzed Borylation

Md Emdadul Hoque, Mirja Md Mahamudul Hassan, Chabush Haldar, Sayan Dey, Saikat Guria, Jagriti Chaturvedi, Buddhadeb Chattopadhyay (2022). ***Synthesis***, 54 (15): 3328 – 3340.

Iridium-catalyzed C-H activation and borylation reaction operate under mild conditions which enable easy and atom economical installation of a notably versatile boronate ester group in an arene, heteroarene, or aliphatic molecules. The standard catalytic system for the iridium-catalyzed borylation entails the usage of $[Ir(cod)(OMe)]_2$ as a precatalyst, a bipyridine type ligand and B_2pin_2 or HBpin as a borylating agent. Initially, a bipyridine ligated trisboryl iridium-complex was generated, which enables borylation reaction and the regioselectivity is mainly governed by the steric of the substituent present on the ring. As a result, monosubstituted and 1,2 –disubstituted arenes give a mixture of isomers. Significant efforts of several research groups have helped to triumph over the selectivity issue for directed proximal C-H borylation by introducing the directing group and newly evolved ligands. This short review aims to summarize the recent elegant discoveries of the directed $C(sp^2)$-H and $C(sp^3)$-H borylation by using heterobidentate ligand (P/N-Si, N-B and N-C) coordinated iridium catalyst.

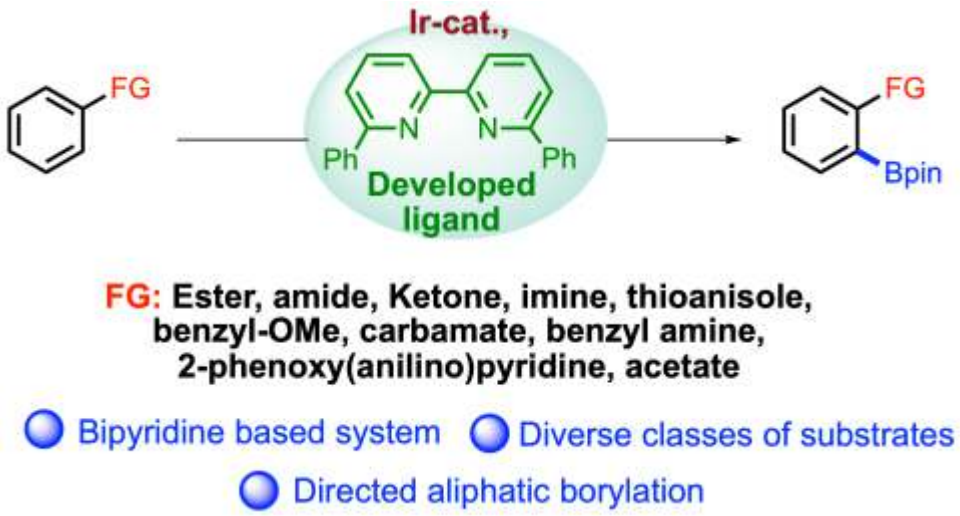


Enabled C–H Borylation of Diverse Classes of Arenes

Ligand Enabled C-H Bipyridine of Diverse Classes Arenes

Md Emdadul Hoque, Sayan Dey, Mirja Md Mahamudul Hassan, Jagriti Chaturvedi, Saikat Guria, Jaitri Das, Brindaban Roy, Buddhadeb Chattopadhyay (2022).
Tetrahedron Chem, 3:100028.

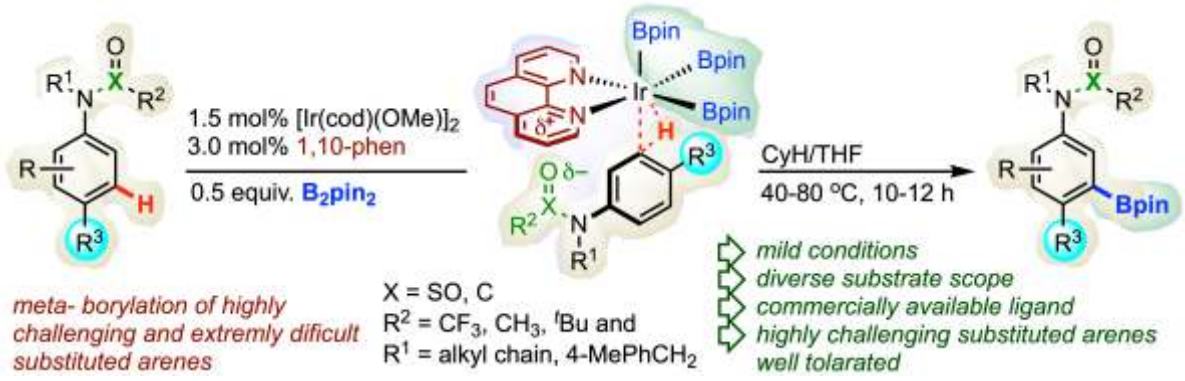
Here we report a new 6,6'-bipyridine based ligand framework for the iridium-catalysed regioselective ortho borylation of diverse classes of arenes containing different functional groups. Moreover, the developed method is highly selective for the directed C(sp^3)-H borylation of the 2-pyridyl amines as well as benzyl and homobenzyl amides directed by pyridine group and amide directed borylation of N-adjacent C-H bond of amides.



Electrostatically Directed *Meta*-Selective Borylation of Arenes

Jagriti Chaturvedi, Chabush Haldar, Buddhadeb Chattopadhyay (2022).
Synlett, 33: 1108-1116.

The constitutional challenge of an electrostatically directed meta-borylation of sterically biased and unbiased substrates is summarized in the present work. The borylation follows an electrostatic interaction between the partially positive and negative charges of the ligand and substrate respectively. Using our developed strategy, it has been demonstrated that a wide range of challenging substrates, especially 4-substituted substrates can selectively be borylated at the meta-position with excellent selectivity. Moreover, unsubstituted substrates are also displayed excellent meta-selectivity. The reaction employs bench stable ligand, proceeds at moderate reaction temperature (40-80 °C) precluding the need to synthesize bulky and sophisticated ligand/template.



Iridium Pyridine-Thienyl Catalyst (Ir-PYT) for C–H Borylation

Md Emdadul Hoque, Mirja Md Mahamudul Hassan, Buddhadeb Chattopadhyay (2022).
Encyclopedia of Reagents for Organic Synthesis (EROS).

Iridium-catalyzed C–H bond activation and borylation is a key method that has attracted remarkable attention due to the versatile synthetic transformation of the C–B bond. The boron functionality in organoboronate esters in principle might be transformed to virtually all functional groups, which makes this borylation chemistry an exceptional method and has considered now as one of the most important mainstream reactions. The standard catalytic system involves the employment of $[Ir(cod)OMe]_2$precatalyst, a bipyridine type of ligand, and bis(pinacolato)diboron as the borylating reagent, which in situ generates a tris(boryl)Ir-complex to facilitate the C–H borylation reaction. But, controlling the site selectivity is one of the major challenges in C–H borylation reactions, except for substrates that usually undergo borylation under sterically directed way. To address this issue, several pioneering concepts have been reported for the proximal ortho as well as remote meta and para selective borylation reactions based on catalyst structure modifications via either directed ortho borylations or by the use of several noncovalent interactions for the remote C–H borylations. Notably, although many methods are now available for the site selective C–H borylation reactions of various substrates using a variety of reaction conditions, the use of a particular set of reaction conditions for each type of substrate class among the diverse class of substrates significantly limits the scope of the borylation reactions. For instance, the coordinating ability of each functional group or the directing group of the substrates is highly dependent on specific transition metals, ligands and other parameters. As a result, for each type of substrates-bearing a specific FG/DG demands independent catalyst design and directing group optimizations in each case that is an extraordinary challenge. Besides, substrates that do not have either proper functional groups or directing groups are really difficult for the site selective C–H borylation. Additionally, the availability of stable Ir-based catalysts for the C–H borylation reactions, which can cover a diverse class of substrates are still uncommon. The catalysts such as, 1st Generation Ir-PYT (**CB1: 1st generation catalyst**) and 2nd Generation Ir-PYT catalyst (**CB2: 2nd generation catalyst**) as well as PYT ligand (**Pyridine-Thienyl Ligand**) have been the authors' contribution to this area of C–H borylation chemistry that have demonstrated remarkable efficiency toward the site selective borylation of a diverse class of substrates, which include, aromatic, heteroaromatic and aliphatic substrates.

Leveraging the Domino Skeletal Expansion of Thia-/Selenazolidinones via Nitrogen-Atom Transfer in HFIP: Room Temperature Access to Six-Membered S/Se,N-Heterocycles

Vandana Jaiswal, Mangilal Godara, Dinabandhu Das, Vincent Gandon, Jaideep Saha (2022). ***The Journal of Organic Chemistry***, 87 (1): 613–627.

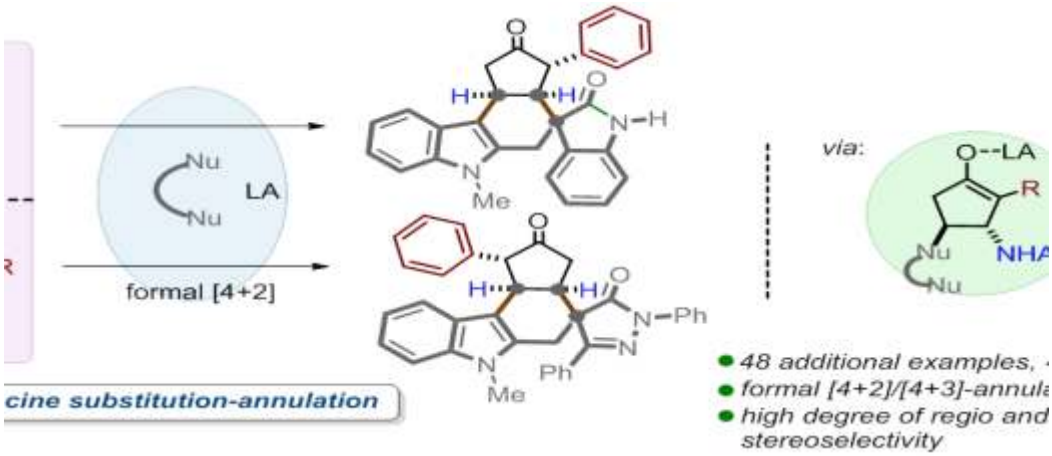
Herein, a highly regioselective domino skeletal-expansion process that transforms 2-aminothiazolidinone into six-membered S,N-heterocycle, is developed with the aid of TMS-azide in hexafluoroisopropanol (HFIP) at ambient temperature. Functioning of the C2 tertiary amine as latent reactive group on the thiazolidinone moiety was central to this development which allowed relay substitution with azide and imparted subsequent ring-expansion under metal/acid free-conditions. Absence of any intermediary azidothiazolidinone in reaction medium characterizes the nitrogen-atom transfer from TMS-azide to final products as a traceless process. The strategy was extendable to analogous synthesis of Se,N-heterocycles and furthermore, late-stage drug-modification and follow-up transformations were also permitted. DFT calculations and control experiments provided important mechanistic insights and highlighted potential roles of HFIP in the transformation.

Skeletal Expansion of Thia-/Selenazolidinones via Nitrogen-Atom Transfer in HFIP: Room Temperature Access to Six-Membered S/Se,N-Heterocycles

An Acid Promoted Pseudocine Substitution Manifold of γ-Aminocyclopentenone Enables Divergent Access to Polycyclic Indole Derivatives

Biplab Mondal, Chenna Jagadeesh, Dinabandhu Das, Jaideep Saha
(2022). ***Chemical Communications***, 58 (15): 2504-2507.

The present work demonstrates γ-aminocyclopentenones as suitable surrogate for reactive cyclopentadienone via *pseudocine*-substitution manifold which enables its orchestrated annulation with tailored bis-nucleophiles and furnish complex β,γ-annulated cyclopentanoids or indole-based polycyclic architectures. This represents a generalized means for direct, regio- and stereoselective β,γ-functionalization of mono or unsubstituted aminocyclopentenones.

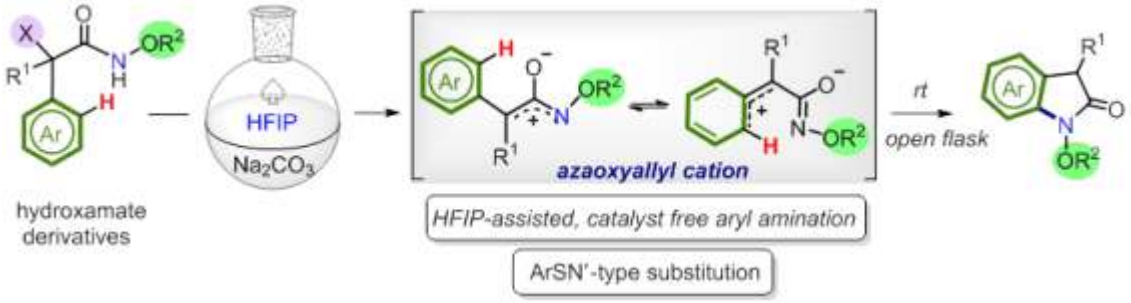


Divergent Access to Polycyclic Indole Derivatives via An Acid Promoted Pseudocine Substitution Manifold

Experimental and Theoretical Investigation of an Azaoxyallyl Cation-Templated Intramolecular Aryl Amination Leading to Oxindole Derivatives

Tishyasoumya Bera, Bandana Singh, Vincent Gandon, Jaideep Saha
(2022). ***Chemistry - A European Journal***, 28 (62): e202201208.

Herein, we disclose the development and detailed investigation of the S_N'-type intramolecular aromatic substitution reaction involving the α-aryl azaoxyallyl cation intermediate. The study showcased that while α-aryl-α-chlorohydroxamates could be activated into the corresponding azaoxyallyl cations, their conversion into π-extended species involving an adjacent α-aryl moiety exhibited a high degree of dependency on the electronics of the aromatic ring as well as on the α-substituents. An effective activation of the α-aromatic ring could pave the path to intramolecular Ar(Csp^2)-N bond formation towards oxindoles. Control experiments and DFT calculations suggested that a non-pericyclic nucleophilic amination pathway is most likely operative and precluded the possibility of concerted or electrophilic amination mechanisms. HFIP as the reaction solvent plays a crucial role in this manifold.

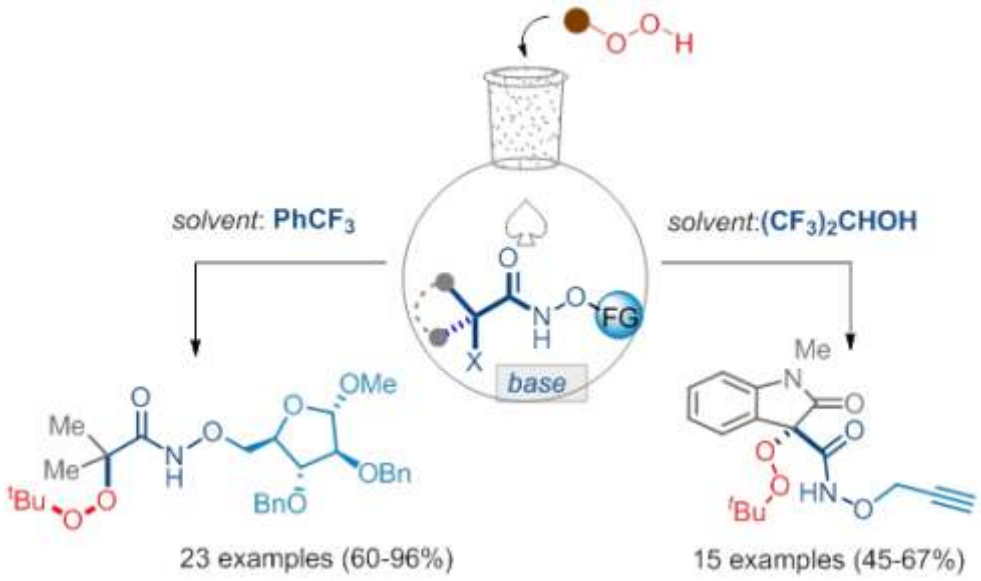


Azaoxyallyl Cation-Templated Intramolecular Aryl Amination Leading to Oxindole Derivatives

Access to 3,3′-Disubstituted Peroxyoxindole Derivatives and α-Peroxyamides via Azaoxyallyl Cation-Guided Addition of Hydroperoxides

Tishyasoumya Bera, Bandana Singh, Manoranjan Jana, Jaideep Saha (2022). ***Chemical Communications***, 58 (54): 7538-7541.

Herein, a metal-free approach for the access to 3,3'-disubstituted peroxyoxindole is disclosed which harnesses transient azaoxyallyl cation. The strategy is also applicable to the synthesis of structurally diverse α-peroxycarboxylic acid surrogates. The method exhibits good functional group tolerance and should push the boundaries of unexplored chemical space for peroxy-containing compounds.

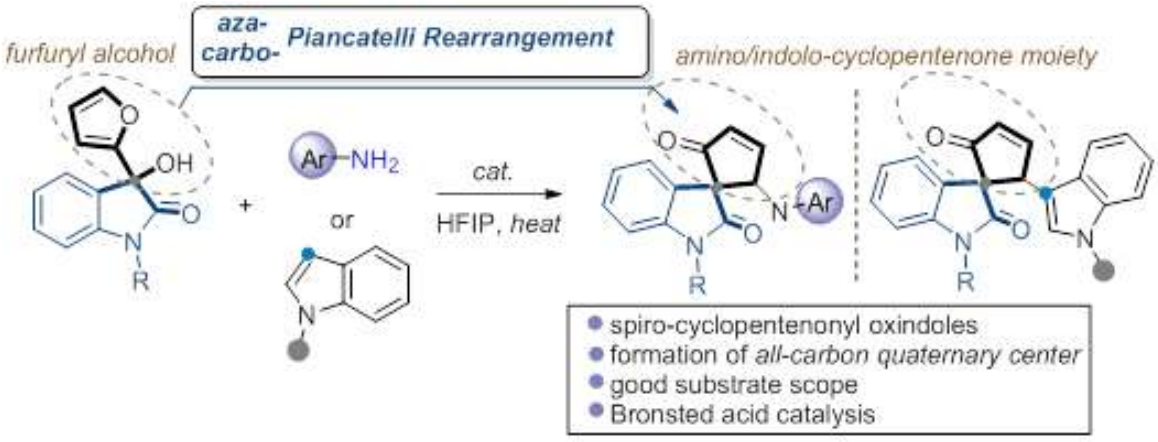


CAPTION: Access to 3,3′-Disubstituted Peroxyoxindole Derivatives and α-Peroxyamides

Access to Densely Functionalized Spirocyclopentenonyl Oxindole Frameworks via aza- and carbo-Piancatelli Rearrangement

Sourav Pramanik, Chenna Jagadeesh, Ayan Chatterjee, Subhas Chandra Debnath, Jaideep Saha (2022).
Organic & Biomolecular Chemistry, 20 (26): 5249 – 5253.

A new means for the access to spirocyclopentenonyl oxindole frameworks is disclosed. In this study an assembly of suitably anchored furfuryl alcohol unit to C3 of an oxindole was used for the development of aza-Piancatelli rearrangement, which furnished the corresponding spirocyclic aminocyclopentenone frameworks. Catalytic phosphomolybdic acid in 1,1,1,3,3,3-hexafluoro-2-propanol (HFIP) was found as the effective promoter for the reaction. Scope of the transformation has been extended to carbo-Piancatelli rearrangement with various indole derivatives. This development is expected to push the boundary of unexplored chemical space of spirocyclopentane oxindole-based structures.

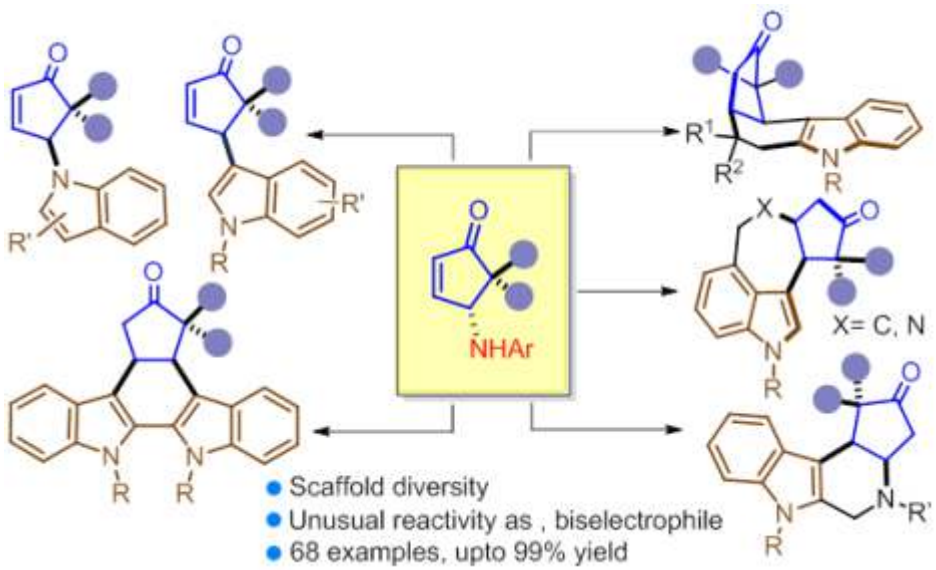


Access to Densely Functionalized Spirocyclopentenonyl Oxindole Frameworks

Development of an Aza-Piancatelli-Templated Reaction Manifold from 4-Aminocyclopentenones: Access to Complex Carbocyclic Assemblies

Chenna Jagadeesh, Biplab Mondal, Jaideep Saha (2022). ***Synlett***, 33 (10): 913-918.

Capitalizing on the propensity of 1,2-amino group migration in γ-aminocyclopentenone with a suitable promoter, gem-diaryl-equipped systems unfolded an unprecedented avenue for the Lewis acid promoted displacement of γ-aniline group with nucleophiles such as indole. Such transformation, besides providing a means for direct γ-functionalization of cyclopentenones, presented innumerable scope for β,γ-annulation. Various tailored indolo bisnucleophiles were explored in the current study that rendered an array of indole alkaloid-like compounds in excellent yields and selectivity through one-pot operation. Analysis of collective experimental observation along with designed control experiments strongly suggested the possibility of a retro aza-Piancatelli rearrangement, which is hitherto unknown in the context. Such repertoire could find potential applications in the synthesis of complex assemblies from the Piancatelli rearrangement and related processes.

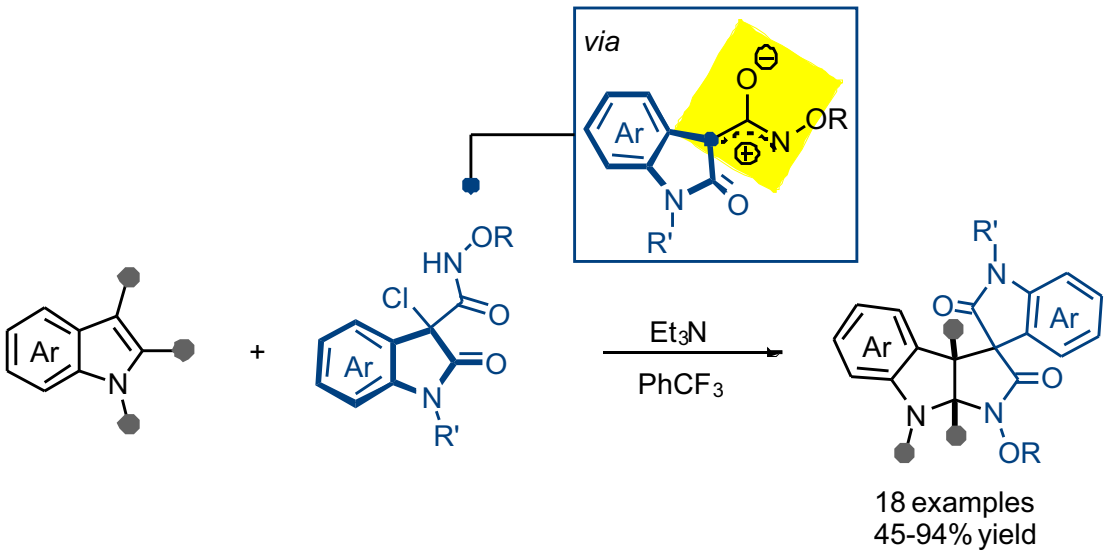


Aza-Piancatelli-Templated Reaction Manifold from 4-Aminocyclopentenones

Construction of Spiro-Pyrroloindolines via Dearomative [3+2]- Cycloaddition of Indole with Oxindole-Embedded Azaoxyallyl Cation

Bandana Singh, Tishyasoumya Bera, Vinod P. Singh, Priyasha Priyasha, Dinabandhu Das, Jaideep Saha (2022). ***Synlett***, 34 (05): 465-470.

Herein, [3+2] dearomative indole cycloaddition reaction with oxindole embedded azaoxyallyl cation at C3 is developed. Use of this new class of azaoxyallyl cation species in the reaction enables the access to more elaborate hexahydropyrrolo[2,3-b]indole moieties that contain a spirooxindole ring. The transformation highlights good substrate scope and good regio- and stereoselectivity for cycloaddition step. Several observations suggested that this class of azaoxyallyl cation can display different reactivity pattern from the commonly employed azaoxyallyl cation systems in the relevant literature.

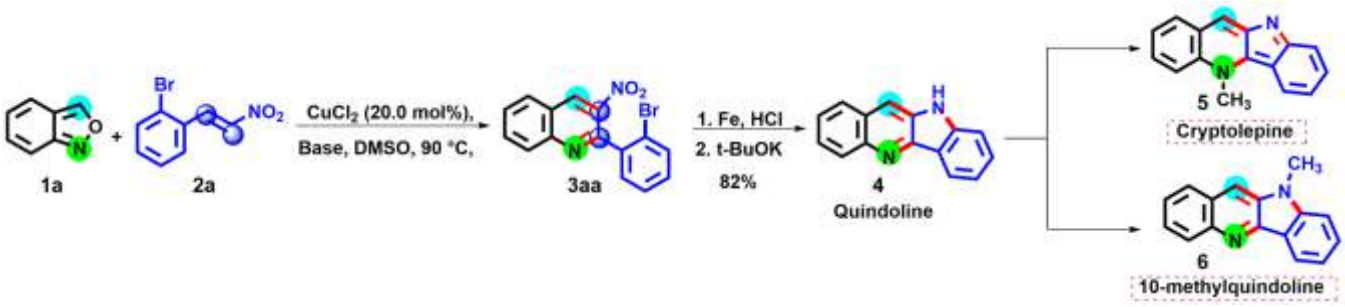


Dearomative [3+2]- Cycloaddition of Indole with Oxindole-Embedded Azaoxyallyl Cation

Copper-Catalyzed Synthesis of 3-Nitro-Quinolines from Nitro-Olefins and Anthranils: Its Application in the Synthesis of Quindoline

Annapurna Awasthi, Pushpendra Yadav, Sourabh Yadav, Dharmendra Kumar Tiwari (2022).
Advanced Synthesis & Catalysis, 364: 41-46.

Quinolines or benzo[b]pyridines are considered to be the most abundant class of nitrogen-containing heterocycles because of their frequent appearance in various natural products, pharmaceuticals, useful ligands, and functional materials. In particular, substituted quinolines with a nitrogen atom in the 3-position are an important key structure for several pharmacologically active substances that have a wide range of biological activities, such as antibacterial, antituberculosis, and EGFR-TK and bis-amide HDAC inhibitor activities. In addition, 3-nitro-quinoline is also used as a synthetic intermediate for the synthesis of various 3-aminoquinolines that are of medicinal relevance. Our current research aims to develop new methods for the synthesis of pharmaceutically important heterocycles. In continuation of the same research program which uses anthranil as the starting material, we report here our latest findings on the copper catalyzed [4+2] cycloaddition reaction between nitro-olefins and anthranils to prepare a wide range of medicinally relevant 2-aryl-3-nitroquinolines. This reaction proceeds through sequential amination, annulation, and oxidation cascades which include the cleavage of N–O bond and the formation of a new C-C and a C-N bond respectively. It is important to mention that, surprisingly, the reaction between 3-nitrostryene and anthranil has not been explored till date.

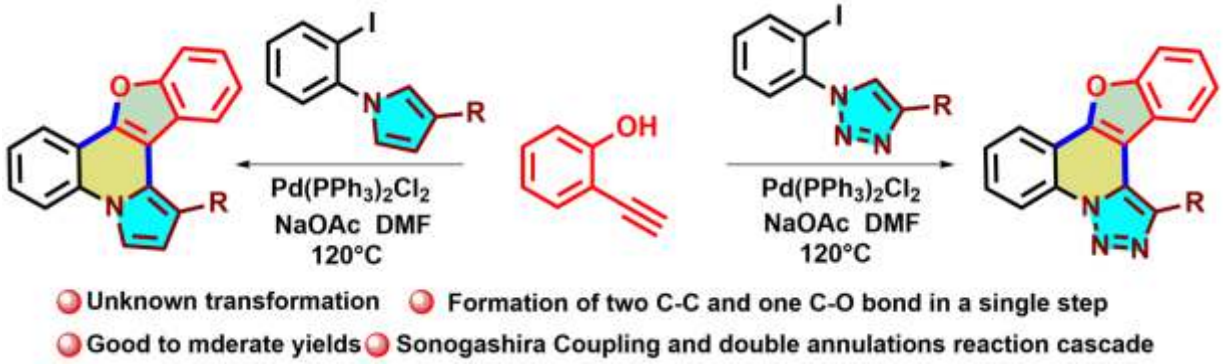


Copper-Catalyzed Synthesis of 3-Nitro-Quinolines from Nitro-Olefins and Anthranils: Its Application in the Synthesis of Quindoline

Pd-Catalyzed One-pot Sequential Sonogashira Coupling and Dual Annulations Cascade for the Synthesis of Benzofuro[3,2-c]-Triazalo/Pyrrolo-Quinolines

Dipak B.Deokar Soumi Laha, B. Sridhar, Dharmendra Kumar Tiwari, and Pravin R.Likhar (2022).
Advanced Synthesis & Catalysis, 364 (22): 3867-3873.

In recent times, transition-metal-catalyzed cascade/tandem reactions have emerged as a powerful tool for the construction of various heterocycles, pharmaceuticals, complex molecules, and natural-product-like scaffolds. These reactions usually rely on an intriguing selectivity, atom economy, and an excellent ability to trigger π systems, especially alkynes, to form intermolecular and intramolecular C-C and C-N bonds. Among various transition metals, palladium-catalyzed tandem reactions have received much attention because of their exceptional reactivity, tolerance of many functional groups, low toxicity, and attractiveness from the viewpoint of assembly efficiency. Now it is well illustrated in the literature that most marketed drugs, pharmaceuticals, and electronic products contain at least one heterocyclic nucleus of quinoline, furan, pyrrole, or triazole.[7] In the recent past, the linking of two different heterocyclic units remains an important transformation in organic synthesis and as a result various furo[3,2-c]quinoline, pyrrolo[1,2-a]quinoline, and [1,2,3]triazolo[1,5-a]quinoline polycyclic compounds have been synthesized and their biological activities against various diseases have been well demonstrated.[8] However, to the best of our knowledge, the examples of molecules containing complex functionalities such as benzofuro[3,2-c]pyrrolo[1,2-a]quinoline or benzofuro[3,2-c] [1,2,3]triazolo[1,5-a]quinoline are unknown till date. Therefore, the development of efficient, convenient, and practical methods to construct this skeleton would open a window for the screening of these materials in medicinal chemistry.

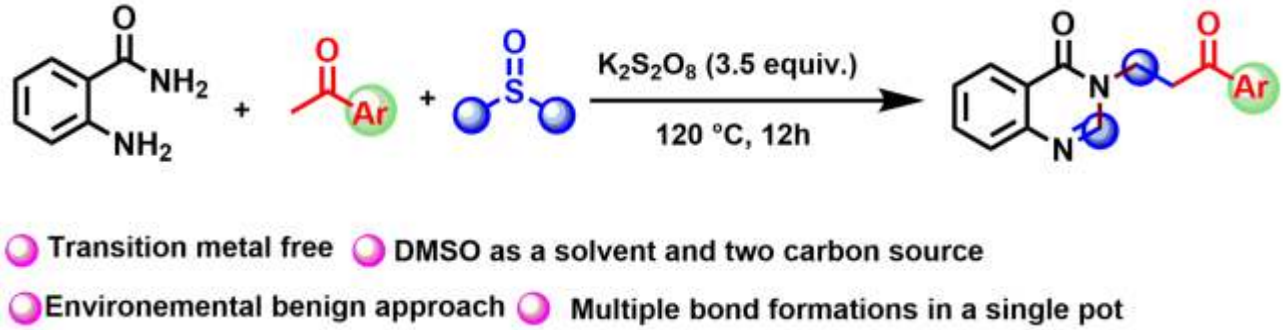


Caption: Pd-Catalyzed One-pot Sequential Sonogashira Coupling and Dual Annulations Cascade for the Synthesis of Benzofuro[3,2-c]-Triazalo/Pyrrolo-Quinolines

DMSO as a Dual Carbon Synthon in One-pot Tandem Synthesis of N-alkylated Quinazolinones from Anthranilamides and Acetophenones:

Pushpendra Yadav , Sourabh Yadav , Annapurna Awasthi , Phanindrudu Mandalparthi, Suman Bhowmick , Dharmendra Kumar Tiwari (2022). ***New Journal of Chemistry***, 46: 16289 – 16296.

Quinazolinones are considered to be the most privileged scaffolds of the aza-heterocycle family. It has attracted considerable interest due to its frequent occurrence in a plethora of biologically important natural products and FDA-approved drugs associated with a wide range of pharmacological activities In the recent past, quinazolinone derivatives have found wide application in the Materials chemistry in the form of fluorescent probes and biological imaging reagents due to their good luminescent properties. They also serve as useful building blocks in the construction of various medicinally active entities. 11 In continuation of our current research program that specifically uses DMSO as a carbon synthon10 we report herein, that DMSO is a dual-carbon source in the synthesis of N-alkylated quinazolinones from readily available anthranilamide and acetophenones under transition metal-free conditions. In this method DMSO is being used as a solvent as well as a two-carbon source, thereby playing a dual role. The reaction proceeded through in situ generations of iminium cation, α,β-unsaturated ketones, followed by oxidative annulation and subsequent aza-Michael addition reaction cascades in a single pot.



Caption: DMSO as a Dual Carbon Synthon in One-pot Tandem Synthesis of N-alkylated Quinazolinones from Anthranilamides and Acetophenones

Df(h22q11)/+ mouse model exhibits reduced binding levels of $GABA_A$ receptors and structural and functional dysregulation in the inhibitory and excitatory networks of hippocampus

Abdel-Rahman Al-Absi, Sakeerthi Kethees Thambiappa, Ahmad Raza Khan, Simon Glerup, Connie Sanchez, Anne M Landau, Jens R Nyengaard (2022). ***Molecular and Cellular Neuroscience***, 122: 103769.

The 22q11.2 hemizygous deletion confers high risk for multiple neurodevelopmental disorders. Inhibitory signaling, largely regulated through $GABA_A$ receptors, is suggested to serve a multitude of brain functions that are disrupted in the 22q11.2 deletion syndrome.

We investigated the putative deficit of $GABA_A$ receptors and the potential substrates contributing to the inhibitory and excitatory dysregulations in hippocampal networks of the Df(h22q11)/+ mouse model of the 22q11.2 hemizygous deletion. The Df(h22q11)/+ mice exhibited impairments in several hippocampus-related functional domains, represented by impaired spatial memory ansensory gating functions. Autoradiography using the [^{3}H]muscimol tracer revealed a significant reduction in $GABA_A$ receptor binding in the CA1 and CA3 subregions, together with a loss of $GAD67^+$ interneurons in CA1 of Df(h22q11)/+ mice. Furthermore, electrophysiology recordings exhibited significantly higher neuronal activity in CA3, in response to the $GABA_A$ receptor antagonist, bicuculline, as compared with wild type mice. Density and volume of dendritic spines in pyramidal neurons were reduced and Sholl analysis also showed a reduction in the complexity of basal dendritic tree in CA1 and CA3 subregions of Df(h22q11)/+ mice.

Overall, our findings demonstrate that hemizygous deletion in the 22q11.2 locus leads to dysregulations in the inhibitory circuits, involving reduced binding levels of $GABA_A$ receptors, in addition to functional and structural modulations of the excitatory networks of hippocampus.

Research Output Indicators

Research Publicaions

Impact Factor (IF)	2022
> 60	01
> 15	02
> 10	03
> 5	18
< 5	44
Not Available	03
Total Papers	71
Average IF	5.73

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65. Jagriti Chaturvedi, Chabush Haldar, Buddhadeb Chattopadhyay (2022). Electrostatically Directed Meta-Selective Borylation of Arenes. ***Synlett***, 33: 1108-1116.

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67. Chenna Jagadeesh, Biplab Mondal, Jaideep Saha (2022). Development of an Aza-Piancatelli-

Templated Reaction Manifold from 4-Aminocyclopentenones: Access to Complex Carbocyclic Assemblies. ***Synlett***, 33 (10): 913-918.

68. Bikash Baishya, Rajeev verma, Rashmi Parihar (2022). Spatially Encoded Polarization Transfer for Improving the Quantitative Aspect of $^{1}H–^{13}C$ HSQC. ***Journal of Magnetic Resonance Open***, 12-13: 100063.

69. Md Emdadul Hoque, Mirja Md Mahamudul Hassan, Buddhadeb Chattopadhyay (2022). Iridium Pyridine-Thienyl Catalyst (Ir-PYT) for C–H Borylation. ***Encyclopedia of Reagents for Organic Synthesis (EROS)***.

70. Amit Mondal, Nirmal Saha, Syed Masood Husain (2022). Concise Chemoenzymatic Total Synthesis of (−)-Rubroskyrin, (−)-Deoxyrubroskyrin (−)-Luteoskyrin, and (−)-Deoxyluteoskyrin. ***Tetrahedron Chem***, 3: 100030.

71. Pranesh Kumar, Mohit kumar, Anurag Kumar Gautam, Archana Bharti Sonkar, Abhishek Verma, Amita Singh, Raquibun Nisha, Umesh Kumar, Dinesh Kumar, Tarun Mahata, Bolay Bhattacharya, Biswanath Maity, Abhishek Pandeya, Sunil Babu Gosipatala, Sudipta Saha (2022). Ameliorative Effect of Fluvoxamine Against Colon Carcinogenesis via COX-2 Blockade with Oxidative and Metabolic Stress Reduction at the Cellular, Molecular and Metabolic Levels. ***BBA Advances***, 2: 100046.

Edited Books

Title: The Coronavirus Pandemic and the Future: Virology, Epidemiology, Translational Toxicology and Therapeutics (Volume 1 & 2)

Editors: Michael D Waters, Alok Dhawan, Tim Marrs, Diana Anderson, Stafford Warren and Claude L Hughes

Publisher: Royal Society of Chemistry, UK, under its series on Issues in Toxicology.

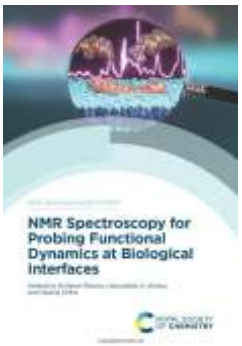
ISBN: 978-1-83916-306-7, 2022.

Title: NMR Spectroscopy for Probing Functional Dynamics at Biological Interfaces

Editors: Anirban Bhunia, Hanudatta S. Atreya, Neeraj Sinha

Publisher: Royal Society of Chemistry, UK

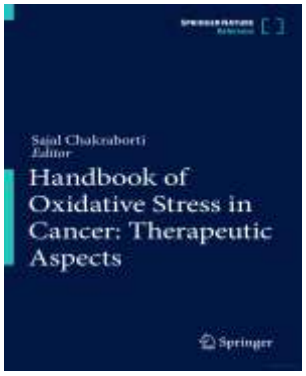
ISBN: 978-1-83916-209-1, 2022.



Book Chapters

1. Garima Kumari, Ashish Guleria, Kulvinder Singh, Nitesh Kumar, Anupam Guleria, **Dinesh Kumar** and Eder Lima (2022). Lignocellulosic biopolymers as potential biosorbents. In ***Biomass, Biofuels, Biochemicals –Biochemicals and Materials Production from Sustainable Biomass Resources***, Editors: Hu Li, S. Saravanamurugan, Ashok Pandey, Sasikumar Elumalai, Publisher- Elsevier, Chapter – 15, pp 391-429, ISBN - 978-0-12-824419-7.

2 Sreemoyee Chakraborti, Adele Stewart, **Biswanath Maity** (2022). Impact of chemotherapeutic drugs towards oxidative stress and associated multiorgan physiological responses. In ***Handbook of Oxidative Stress in Cancer: Therapeutic Aspects***, Editor: Sajal Chakraborti, Publisher-Springer, Chapter – 199, pp 3961-3985, ISBN -978-981-16-5421-3, 978-981-16-5422-0 (eBook).



3. **Alok Dhawan,** Claude Hughes, Timothy Marrs, Stafford Warren, Michael Waters and Diana Anderson. The COVID-19 pandemic: global lessons for the future. In ***The Coronavirus Pandemic and the Future: Virology, Epidemiology, Translational Toxicology and Therapeutics,*** Editors: Michael D Waters, Alok Dhawan, Tim Marrs, Diana Anderson, Stafford Warren, Claude L. Hughes. Publisher - Royal Society of Chemistry, UK (2022). Chapter- 24, Volume 2, pp. 604-624, ISBN-978-1-83916-306-7.

4. Richa Dubey and **Neeraj Sinha**. Structure and dynamics of native biological materials by solid-state NMR spectroscopy. In ***NMR Spectroscopy for Probing Functional Dynamics at Biological Interfaces***, Editors: Anirban Bhunia, Hanudatta S Atreya, Neeraj Sinha. Publisher-Royal Society of Chemistry 2022. Chapter-21, pp.614-646, ISBN-978-1-83916-209-1.

Patents filed

S.No.	Title	Inventors	Filing / Granted date	Application Number
1.	A New Ligand Framework for para Borylation of Arenes	Haldar, C.; Bisht, R.; Chaturvedi, J.; Guria, S.; Chattopadhyay B. Status	January 11, 2022	202211001312
2.	A New Ligand Scaffold (PY-PYRI) for the Meta Borylation of Phenol Derivatives	Guria, S., Hassan, M. M. M., Dey, S., Chattopadhyay B.	June 25, 2022	202211036590
3.	A Method for Tandem 1,3-Functionalization of Azabicyclo [1.1.0]-butane to Functionalized Azetidines	Jaiswal, V., Mondal, S., Saha, J	December 22 2022	202211074718
4.	Novel Method for Metal-Free Synthesis of Nitriles from Aldehydes Using N-Boc-O-Tosylhydroxylamine as Nitrogen Source	P. Kumar, V. Singh, J. L. Jat, B. Tiwari.	December, 30 2022	202211077473
5.	Method for Metal-Free Synthesis of Secondary Amides using N-Boc-O-Tosylhydroxylamine as Nitrogen Source via Beckmann Rearrangement	L. Jat, P. Kumar, S. Verma, D. Chandra, V. Singh, B. Tiwari	December, 30 2022	202211077495

Patents granted

S.No.	Title	Inventors	Filing / Granted date	Application Number
1.	Catalyst/Ligand Engineering for C–H Borylation of Diverse Classless of Aromatic and Heteroaromatic Molecules.	Hoque, E., Hassan, M. Chattopadhyay, B.	June 23, 2022	399886
2.	Process for preparing Indeno [1,2-D] Thiazolo[3,2-A] Pyrimidine containing nitrogen-bridgehead	Amit Keshari Sudipta Saha Gosipatala Sunil Babu, Biswanath Maity	September 6, 2022	405884

Ph.D Awarded

Name	Thesis Title	Year	Supervisor	University
Upendra Singh	Development of Ultra-High Resolution NMR Method and its appoleation thesis Abstract	2022	Dr. Bikash Baishya	Banaras Hindu University
Amit Mondal	Chemo enzymatic approach towords the synthesis of Bisanthraquinouns	2022	Dr. Syed Masood Husain	University of Kalyani
Shailesh Kumar Singh	Identification and Characterization of NAD (P) H-Depnendent Oxioreductases and their Applications	2022	Dr. Syed Masood Husain	University of Kalyani
Chabush Haldar	Iridium-Catalyzed site selective C-H Bond Borylation of Arnes and Heteroarenes	2022	Dr. Buddhadeb Chattopadhyay	Banaras Hindu University
Jagriti Chaturvedi	Iridium –Catalyzed C-H Bond Activation and Borylation of Small Organic Molecules	2022	Dr. Buddhadeb Chattopadhyay	BBAU A Central University
Ramkrishna Maity	Asymmetric Total Synthesis of Euplainilide E, Integrifolin and Allied Guaianolides	2022	Professor Saumen Hajra	Banaras Hindu University

Ongoing Extramural Projects

S. N.	Principal Investigator (PI)	Project Title	Funding Agency	Duration of Project	Amount (In ₹)
1.	Dr. Bhoopendra Tiwari	First Direct Enantioselective Synthesis of Unactivated Aziridines from Enals and Indoles	SERB	2019-2022	51.66
2.	Dr. Ahmad Raza Khan	Novel and Translational biomarkers for Early Detection of Repetitive Mild Traumatic Brain Injury	DBT	2019-2024	113.60
3.	Dr. Buddhadeb Chattopadhyay	C-H Borylation via Attractive Weak Interactions	SERB	2020-2023	38.50
4.	Dr. Buddhadeb Chattopadhyay	Concept of Catalyst Engineering for Borylation of Small Organic Molecules	SERB	2020-2023	77.35
5.	Dr. Dharmendra Kumar Tiwari	Transition Metal Free One-Pot Tandem Synthesis of Medicinally Relevant N-Heterocycles Using DMSO as Carbon Source	SERB	2020-2023	44.52
6.	Prof. Saumen Hajra	Asymmetric Total Synthesis of Anticancer Compounds – 3α – O - (β-D-Glucopyranosyl) desoxypodophyllotoxin, Propolisbenzofuran B and More	SERB	2020-2023	63.33
7.	Dr. Jaideep Saha	Investigation on the Expansion of Application Portfolio of Oxyallyl Cation and Related Species from Complex Molecular Synthesis to Site-Selective Protein Modifications	SERB	2020-2023	49.93
8.	Dr. Biswanath Maity	Atypical G Protein Regulator Might be Developed as Novel Target to Attenuate Chemo Induced Hypertrophy Through CaMKII Dependent T Tubule Remodeling	DBT	2020-2023	68.00
9.	Prof. Saumen Hajra	Asymmetric Total Synthesis of Eupalinilide E and Allied Guaianolides	CSIR	2021-2024	33.92
10.	Dr. Syed Masood Husain	Chemoenzymatic, Asymmetric, Total Synthesis of Nodulones and Their Non-Natural Analogs Using a Fungal Oxidoreductase Enzyme and its Biosynthetic Implications	CSIR	2021-2024	33.50
11.	Dr. Ashish Gupta	Analogue of Prothrombin Time: Identification and Assay Development of Novel Non-Invasive and Surrogate Indicator of Blood Coagulopathy	ICMR	2021-2024	40.03

12.	Dr. Jaideep Saha	Exploring Dual Activation Strategies Using Transient Azaoxyallyl Cations: New Opportunity for Heterocycle Synthesis	CSIR	2021-2024	29.60
13.	Dr. Uttam Kumar	Tactile Perceptual Processing in	DST	2021-2024	59.61
14.	Neeraj Sinha	Indo – Japan workshop on Magnetic Resonance Deaf: fMRI Study	DST	2022-2023	9.50
15.	Dr. Biswanath Maity	R7RGS-Gβ5 Complex can be Developed as a Novel Target to Attenuate Chemotherapeutic Induced Hypertrophy to Heart Failure Transition through Nox-ROS-CaMKII-T Tubule Remodeling	ICMR	2021-2024	95.00
16.	Dr. Syed Masood Husain	Biocatalytic Method for the Asymmetric Synthesis of Pharmaceutically Important substituted Benzodiazepines, Benzoxazepines and Benzothiazepines using Imine Reductases	SERB	2022-2025	48.42
17.	Dr. Bhoopendra Tiwari	First Direct Access to (Hetero) Functionalized Enantioenriched Pyrazolines and Isixazolines using Hypervalent Iodine Catalysis	SERB	2022-2025	38.70
18.	Dr. Buddhadeb Chattopadhyay	Noncovalent Catalysis and Ligand Design for Borylation of Small Organic Molecules	SERB	2022-2025	79.63
				TOTAL (In ₹)	**974.80**

Honours and Awards

Professor Alok Dhawan
Director

- Listed among top 2% scientists of the world as published by Stanford University in the article: Ioannidis, John P.A. (2022), "September 2022 data-update for (Updated science-wide author databases of standardized citation indicators);", Mendeley Data, V4, doi: 10.17632/btchxktzyw.4 (October 10,2022)
- BHU Centennial Award 2021 of The Biotech Research Society, India for outstanding contributions in Nanomaterial Toxicology and Life Sciences. (December 7, 2022)
- Chairman, Scientific Panel on Contaminants in Food Chain, FSSAI, GoI.
- Chairman, Working Committee for drafting UP-Science & Technology Innovation Policy constituted by Department of Science & Technology, Government of Uttar Pradesh, 2022
- Member, Indian Delegation in Codex Committee on Contaminants in Foods (CCCF15), virtually from May 9-13, 2022.
- Member, Scientific Advisory Committee, ICMR- National Animal Resource Facility for Bio- Medical Research, Hyderabad. 2021-2022
- Chairman, Institutional Ethics Committee, King George's Medical University, Lucknow. 2021-2023

Dr. Saumen Hajra
Professor

- Member, Program Advisory Committee (PAC)- Organic Chemistry, SERB, DST, GoI (2021-2024)
- Member, Research Committee, SGPGIMS (2020-2023)

Dr. Bikash Baishya
Associate Professor

- Professor S. Subramanian's 60th Birthday Lecture Award – 2022 instituted by the National Magnetic Resonance Society (NMRS), India

Dr. Dinesh Kumar
Associate Professor

- Associateship of Indian Academy of Sciences (IASc) for three Years (2019 – 2022)
- Member of National Academy of Sciences India (NASI) in Biological Sciences section

Dr. Buddhadeb Chattopadhyay
Associate Professor

- SERB-TETRA AWARD–2022" (Technology Translation Award)

EVENTS

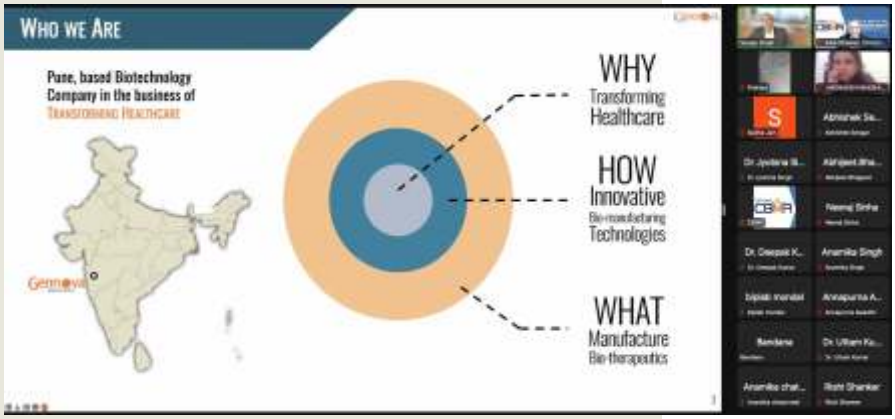
National Science Day

February 28, 2022

Dr. Sanjay Singh

Chief Executive Officer
Gennova Biopharmaceuticals Ltd, Pune

Dr. Sanjay Singh delivered an online lecture on the integrated approach in science and Technology, with a focus on need-based innovation and how scientific advancements have been able to conquer dreaded diseases in India. He also provided examples of how India was able to manage the COVID-19 pandemic through the indigenous development of vaccines and testing kits.



21st Governing Council Meeting

March 05, 2022

The 21st Governing Council/General Body meeting of CBMR was held on March 05, 2022 in the Board Room under the Chairmanship of President, CBMR/Chief Secretary, Government of Uttar Pradesh, Shri Durga Shanker Mishra.

Dr Sanjeev Misra, Director, AIIMS Jodhpur; Dr C.M. Gupta, Chairman, SAC; Shri Alok Kumar, Principal Secretary, Medical Education Department, Govt. of U.P; Dr Anurag Agrawal, Director, CSIR-IGIB, New Delhi; Dr R.S. Dhaliwal, Scientist 'G' & Head, Non Communicable Diseases (NCD) Division, ICMR Hq, New Delhi; Professor R.K. Dhiman Director, SGPGIMS; Professor Jayesh Bellare, Institute Chair Professor, IIT-Bombay; Dr Sanjay Singh, CEO, Gennova Biopharmaceuticals Ltd., Pune; Shri Anupam Jalote, CEO, iCreate, Ahmedabad; Shri Pavitra Kumar, Joint Secretary, Finance Department, Govt. of U.P.; Professor Alok Dhawan, Director, CBMR, Lucknow, Dr Anil Kumar Mishra. Director, DRDO-INMAS, Delhi; Professor Neeraj Sinha, Dean, CBMR and Shri P.D. Upadhyay, Finance Controller, CBMR attended the meeting.

L – R: Professor Neeraj Sinha, Dean, CBMR; Dr. Anil Kumar Mishra, Director, DRDO-INMAS, Delhi, Professor Alok Dhawan, Director, CBMR; Shri Durga Shanker Mishra President, CBMR/Chief Secretary, Government of Uttar Pradesh; Dr. Sanjeev Misra Director, AIIMS Jodhpur; Shri Alok Kumar, Principal Secretary, Medical Education Department, Govt. of U.P; Professor R.K. Dhiman, Director, SGPGIMS, Lucknow

National Technology Day

May 11, 2022

Dr. Atul Goel

Senior Principal Scientist
Medicinal & Process Chemistry Division
CSIR - Central Drug Research Institute, Lucknow

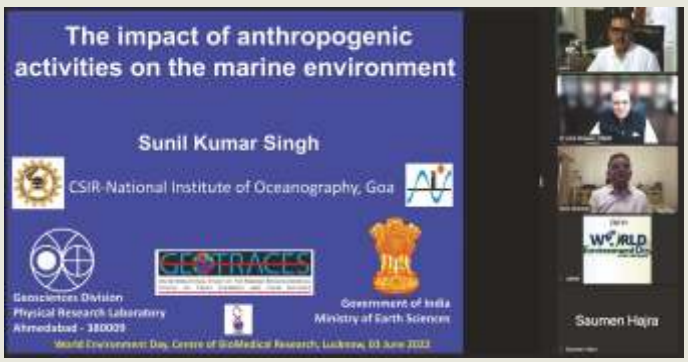
Dr Atul Goel, Sr Principal Scientist, CSIR-CDRI delivered a facinating National Technology Day Lecture on "Development of Fluorescent Probes for Diagnostics and Devices".He shared the various technologies developed by his team at CSIR-Central Drug Research Institute and transferred to industry. He also showed the indigenous RTPCR kit developed for detection of different strains of COVID19.

World Environment Day

June 5, 2022

Professor Sunil Kumar Singh

Director
CSIR - National Institute of Oceanography, Goa



On June 5, 2022, CBMR celebrated World Environment Day to raise awareness and promote actions for the protection and preservation of the environment. Prof. Sunil Kumar Singh, Director, CSIR-National Institute of Oceanography, Goa delivered an insightful lecture on this occasion and apprised the audience of how the anthropogenic activities have altered the marine environment. He also expressed concern of climate change and its detrimental impact on life on planet earth.

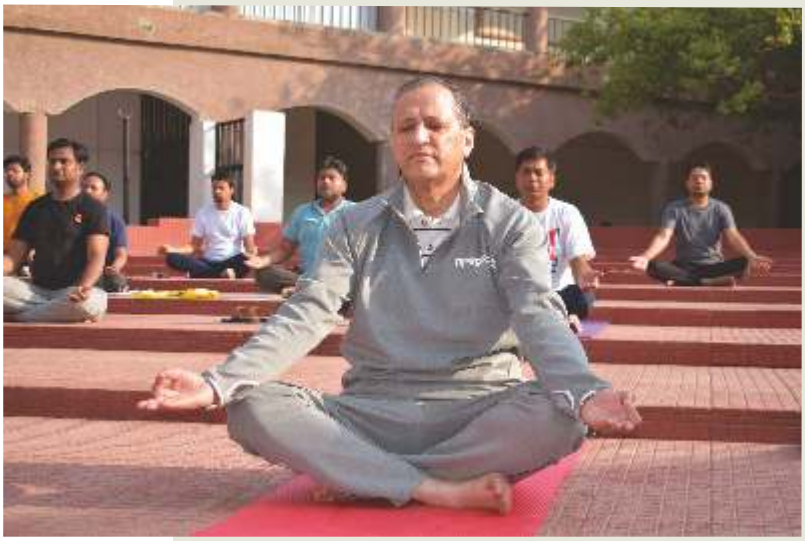
International Day of Yoga

June 21, 2022

In recognition of the ancient practice of yoga and to celebrate its physical and spiritual benefits, June 21 marks International Day of Yoga every year.

On June 21 2022, CBMR celebrated 8th International Day of Yoga under the theme " Yoga for humanisty". The yoga session was conducted in the morning at 6:00 AM at CBMR Campus by the profession yoga trainer Dr Ritu Saxena, who is associated with Bengaluru Art of Living Organisation.

Warm up exercises were taken and all the faculty, staff and students practiced & performed sitting and standing asanas. Dr Saxena simultaneously explained the importance of these asanas. The celebration concluded with the speech of the Director, CBMR. He encouraged faculty, staff and students to practice regular yoga to remain fit and improve concentration.



Independence Week Celebrations

August 11- 17, 2022

Azadi Ka Amrit Mahotsav, an initiative of the Government of India to celebrate and commemorate 75 years of independence and the glorious history of it's people, culture and achievements was celebrated with great fervor. In the year 2022, the Government of Uttar Pradesh decided to celebrate Azadi Ka Amrit Mahotsav as an Independence Week from August 11-17, 2022. The Independence week was celebrated with a great enthusiasm at CBMR during 11-17 August, 2022. Various events such as Table Tennis tournament, prabhat pheri, painting competition for school children, student visit and tree plantation were organised.

Table Tennis

August 11, 2022

A table tennis tournament was organised. The Director, Dean, faculty, staff and students of CBMR participated in the tournament. The faculty and staff members participated in Group-A and PhD and other research scholars participated in Group-B. Mr. Amar Dixit, Administrative officer in Group-A and Mr Saumik Mondal, Research Scholar in Group-B were the winners.

Prabhat Pheri

August 12, 2022

A "Prabhat Pheri" was organised by CBMR on August 12, 2022. Professor Alok Dhawan, Director and all the staff and faculty members along with students marched with tricolours in rows raising slogans including 'Bharat Mata ki Jai', 'Vande Mataram' and 'Har Ghar Tiranga, Har Mann Tiranga'

Children Painting Competition

August 13, 2022

A painting competition was held in the CBMR Campus on August 13, 2022. The children of faculty and staff of CBMR and other nearby schools participated with great enthusiasm portraying their feelings for independence and patriotism.

Flag Hoisting

August 15, 2022

On Independence Day August 15, 2022, Professor Alok Dhawan, Director, CBMR hoisted the Indian Flag and addressed the gathering on the importance of independence, sacrifices of freedom fighters and responsibilities of citizens. He also highlighted the achievements of the Centre and exhorted the scientist to work towards achieving the goals of an Atmanirbhar Bharat.

Tree Plantation

August 17, 2022

Tree plantation is a great way to raise awareness about the importance of trees and the need for environmental conservation. Contributing in this aspect, a tree plantation drive was organized on August 17, 2022. CBMR staff members planted different varieties of trees at the CBMR residential campus.




















Symposium on
Women Driving S&T in India

August 25-26, 2022

WOMEN
Driving S&T in India

A two-day national event on ***"Women Driving Science and Technology in India"*** was organized by the Centre of BioMedical Research (CBMR), Lucknow, under the aegis of the Science and Engineering Research Board (SERB), New Delhi on August 25-26, 2022. It was the first event of its kind in the State of Uttar Pradesh. This event was aimed at providing a platform for PhD students and early career faculty from the state of Uttar Pradesh to get familiar with the existing and/or potential S&T opportunities for women in both academic and corporate sectors of India.

The inaugural function was held on August 25, 2022. Professor Alok Dhawan, Director, CBMR welcomed all the dignitaries, speakers and participants.

Professor Alok Dhawan appraised the participants and speakers about the genesis of the event. He mentioned how institutions should formulate policies for enabling women to take up S&T as a career.

The Chief Guest, **Professor Soniya Nityanand**, Director, RMLIMS inaugurated the event. Professor Shinjini Bhatnagar, THSTI and Dr Ricky Kej, GRAMMY Awardee were the Guests of Honour. Professor Shinjini Bhatnagar in her remarks mentioned that she was fortunate to have mentors who always encouraged her to do the best due to which she achieved great heights both nationally and internationally in her field. She mentioned that one should get out of their comfort zones and look for better opportunities as a priority. Dr Ricky Kej, mentioned that it is important to include women in all spheres of S&T to ensure that they can contribute to the growth and economy of India.

Chief Guest, Professor Soniya Nityanand, Director, RMLIMS, Lucknow delivering the Inaugural Adress

Professor Soniya Nityanand in her remarks gave several examples of women scientists in India who have been outstanding in their fields. Professor Nityanand shared the contributions of Indian women from various disciplines of science and spoke briefly about Dr Anandibai Joshi, Dr Asima Chatterjee, Dr Darshan Ranganathan and others, She exhorted the students and faculty alike to take up problems relevant to their surroundings and align themselves towards the national missions and goals. She said that these days women are contributing equally in S&T as well as medicine and there are immense opportunities in these areas including engineering where the youth should actively engage to ensure that India becomes self-reliant and the topmost economy in the world.

Release of Abstract book of the event "Women driving S&T in India"
L-R: Professor Alok Dhawan, Director CBMR; Dr Ricky Kej, GRAMMY Awardee; Professor Soniya Nityanand, Director, RMLIMS; Professor Shinjini Bhatnagar, THSTI and Professor Neeraj Sinha, Dean, CBMR

Release of a book on The Coronavirus Pandemic and the Future: Virology, Epidemiology, Translational Toxicology and Therapeutics, Volume 1 & 2 published by The Royal Society of Chemistry (RSC), UK
L-R: Mr. Rajesh Parishwad, RSC; Professor Alok Dhawan, Director CBMR; Dr Ricky Kej, GRAMMY Awardee; Professor SoniyaNityanand, Director, RMLIMS; Professor Shinjini Bhatnagar, DBT-THSTI and Professor Neeraj Sinha, Dean, CBMR

The dignitaries on the dais released the Abstract book of the symposium as well as a book on *The Coronavirus Pandemic and the Future: Virology, Epidemiology, Translational Toxicology and Therapeutics, Volume 1 & 2* edited by Michael D Waters, Alok Dhawan, Tim Marrs, Diana Anderson, Stafford Warren, Claude L Hughes and published by The Royal Society of Chemistry, UK.

Professor Neeraj Sinha, Chairman of the symposium proposed a vote of thanks. He thanked the Secretary, SERB for the generous financial support as well as helping in shaping up the programme. He also thanked the speakers as well as participants who attended this symposium. Professor Sinha thanked the faculty and staff of CBMR for organising the symposium so efficiently.

A total of about 200 PhD and early career faculty participated in the conference from institutes including CSIR-CDRI, CSIR-IITR, CSIR-CIMAP, CSIR-NBRI, BSIP-Lucknow, IIT-Kanpur, NIPER-Raebareli, Era University, Amity University-Lucknow, BBAU, Integral University, Lucknow University, Dr Ram Manohar Lohia Institute of Medical Sciences, King George's Medical University, Chhatrapati Shahu Ji Maharaj University etc.

Dr Ricky Kej, 2X GRAMMY® Award Winning Music Composer delivering the Keynote Lecture

Dr Ricky Kej, 2X GRAMMY® Award Winning Music Composer and Environmentalist from Bengaluru delivered an engaging lecture entitled "Music for the Planet". He shared his journey of environmental sustainability through the universal language of music. This will require a change in our lifestyles. Dr Ricky also shared how we need to be mindful of the fact that while we are industrialising and expanding our footprints on the planet, we are losing several species which are important for a balanced ecosystem.

Ms. Nivruti Rai, Country Head, Intel India, spoke on the opportunity for women in the corporate sector and how the young aspirants can keep up their zeal and motivation to achieve their goals. She also shared with the audience her own journey where she was able to balance work and family life. She expressed her keen desire to start some AI based programmes with CBMR.

Ms. Nivruti Rai, Country Head, Intel India, delivering the Keynote Lecture

Theme – 1: Biomedical Research & Ethics

Dr Roli Mathur, ICMR delivering Plenary Lecture

Dr Roli Mathur, ICMR, Bengaluru delivered a plenary lecture on "ICMR Initiative in Bioethics". She shared how her Centre became the first WHO-collaborating unit in the south-east Asia region. She highlighted the importance of bioethics in research and encouraged the women researchers to learn and execute the bioethics principles to generate quality data from their studies.

Professor Shinjini Bhatnagar from DBT-THSTI, Faridabad delivered a plenary lecture. She encouraged the women students present in the audience to pursue an active career in science discipline and shared her journey on the development of the rotavirus vaccine.

A panel discussion that was followed moderated by Professor Shally Awasthi from KGMU & Professor Shinjini Bhatnagar. Dr Alka Sharma from the Department of Biotechnology, Government of India, New Delhi, Dr Deepak Modi from ICMR-NIRRCH Mumbai and Dr Poonam Kakkar were panel members. In this interactive session, several questions from female participants in the audience were addressed by the panelists.

Professor Shinjini Bhatnagar, DBT-THSTI delivering Plenary Lecture

Theme–2: Science Leadership in Basic Sciences for Promoting Sustainable Development

First Plenary Lecture was delivered by **Professor Priya Abraham**, Director, ICMR-NIV Pune on the "Emerging and re-emerging viral diseases – Responses and Challenges". She emphasized how the current pandemic has called upon scientists globally to engage in innovative science Abraham highlighted the role of women scientists and healthcare workers in handling the pandemic

Professor Priya Abraham, Director, ICMR-NIV Pune Plenary Lecture

Dr G. Taru Sharma, DBT-NIAB delivering Plenary Lecture

The session continued with another plenary lecture delivered by **Dr G. Taru Sharma**, Director, DBT-NIAB, Hyderabad on "Women excelling in STEMM to boost knowledge economy" reconnecting that elusive fetal stem cells to basic sciences which ultimately could lead to regenerative therapy. She talked about the contributions of Indian Women in Science and Technology. She exhorted the students to come forwards and leave their comfort zones to take up challenges in animal research. This will not only improve their quality of work but will also make them future ready to take up leadership roles.

Professor Gill Reid, President, The Royal Society of Chemistry (RSC), UK, said Inclusion and diversity are central to advancing excellence in the chemical sciences and shared RSC strategy. The RSC goal of Inclusion and Diversity strategy to 2025 is to increase the diversity of people choosing and fulfilling their potential in the chemical sciences for a truly inclusive community.

She shared that the people thrive in institutions and organisations where they have belongingness, and that diversity of thought, perspective and experience are required for individuals and organisations to be

Professor Gill Reid, President, The Royal Society of Chemistry, UK delivering a Plenary lecture

successful. She highlighted RSC's initiatives and policy work supporting Inclusion and Diversity in chemical Sciences Community such as Careers' Grant and reports such as Breaking the Barriers; Gender bias in publishing and the recent work in India on Gender Diversity.

Professor Ried also announced RSC's collaboration with the Chemical Research Society of India and other partners to publish an evidence-based report on Gender Diversity in the Indian Chemical Sciences research community. The report will strategise a roadmap to address the institutional, organizational & skills gaps in empowering women-researchers in Chemistry in the Indian academic landscape.

These lectures were followed by a panel discussion which was moderated by Directors Dr Geetanjali Sachdeva director ICMR- NIRRCH & Dr Vandana Prasad director DST- BSIP, Lucknow. The panel members were Professor Priya Abraham, ICMR-NIV, Pune and Dr G. Taru Sharma, DBT-NIAB, Hyderabad. In this interactive session, women in leadership served as an example to other fellow women scientists, giving hope that there are multiple avenues and potential S&T opportunities for women in both academic and corporate sectors of India. The panel members recounted the challenges they faced, how they overcame them, and discussed the support system they think organisations can provide to a woman.

Chairpersons and Panelist during the session "Science Leadership in Basic Sciences for Promoting Sustainable Development" L-R: Dr Geetanjali Sachdeva,ICMR- NIRRCH; Dr G. Taru Sharma, DBT-NIAB; Professor Veena Tandon, NASI; Professor Pramod Tandon, Biotech Park; Professor Alok Dhawan, CBMR and Dr Vandana Prasad, DST-BSIP

Theme – 3: Entrepreneurship for an Atmanirbhar Bharat

Dr Jitendra Sharma, AMTZ, delivering a Plenary Lecture

This session was chaired by Professor Alok Dhawan and Professor Shinjini Bhatnagar.

Plenary lectures in this session were delivered by the industry delegates. **Dr Jitendra Sharma** from AMTZ, Visakhapatnam described how AMTZ took a leading role during the COVID pandemic and supported India's need for 12 lakh RT-PCR test kits across the country every day at the peak. He highlighted the opportunities that female aspirants can explore in biotech industries including at AMTZ. Dr Sharma also informed how at AMTZ apart from being a manufacturing hub for startups, has started a programme for skilling young engineers for handling sophisticated equipment. He invited young and enterprising women to join their pool of installation engineers across the country, to ensure that the footprint of Indian Medical Technology in India and in the world grows at an exponential rate with every step that a woman Biomedical Engineer takes.

Dr Janhavi Raut, from Unilever R&D India, Bengaluru spoke on "Of Humans…and Microbes…and Soaps". She presented the science of soap and how fundamental science is supporting the development of newer formulations for over a century. She also mentioned how important hand hygiene was during the pandemic. Dr Raut shared her research activities at Unilever and highlighted the opportunities for women scientists..

Dr. Janhavi Raut, Unilever R&D India, delivering a Plenary Lecture

Dr Kavita Nigam, KARAM Group, delivering a Plenary Lecture

Dr Kavita Nigam, KARAM Group, Lucknow spoke on "Career opportunities for Women in Science & Technology in the Private Sector". She shared the evolving role of women in the manufacturing industry and talked at length on her own career transition from being a medical student which helped her drive innovation in various personal protective devices in her company. Dr Nigam also highlighted the contributions of women as head of Human Resource in industrial setting

A panel discussion was held subsequent to the lectures. Additional industry personnel including **Dr Roli Budhwar** from Bionivid Technology Pvt Ltd, Bengaluru joined as the panel member along with the Plenary Speakers and questions from the audience on various aspects of entrepreneurship were addressed to ensure that the country enables a framework for the success of the entrepreneurs.

Dr Roli Budhwar, Bionivid Technology Pvt Ltd during the Panel discussion

Theme – 4: Technology for Healthcare

This session was chaired by Dr Janhavi Raut, Director, Unilever R&D Bengaluru and Dr G. Taru Sharma, Director, DBT-NIAB, Hyderabad.

Dr Viswajanani J. Sattigeri from CSIR-TKDL, New Delhi presented the first Plenary lecture in this session. Her lecture focused on "Changing Dynamics of Life and Opportunities for Women". She highlighted how women scientists have contributed in compiling and now managing the CSIR-Traditional Knowledge Digital Library which has been opened to the public. She also shared anecdotes from her journey – the ups and downs and talked about the essentials of work-life balance for women in the S&T domain.

Dr Viswajanani J. Sattigeri, CSIR-TKDL delivering a plenary lecture

Dr Swati Subodh, C-CAMP delivering a plenary lecture

The second plenary lecture on "Bridging Silos in Healthcare" was delivered by **Dr Swati Subodh** from C-CAMP, Bengaluru. In her talk, she described how the health needs are transitioning from quick-fix solutions to sustained long-term interventions as age and disease demographics are continuously changing around the globe. She emphasized that silos between the scientific development and deployment of those innovations require to be bridged in order to ensure accessible and equitable healthcare solutions for all.

Later a panel discussion was held which was moderated by Dr Viswajanani J. Sattigeri from CSIR-TKDL and Dr Swati Subodh from C-CAMP and the panelists were Professor Neeraj Sinha from CBMR, Lucknow and **Dr Swapnali Hazarika** from CSIR-NEIST, Jorhat. Main discussion theme was how healthcare technologies have matured over the time and how it has benefited the management of the recent pandemic in India and globally. Questions from the students and participants from various institutions were addressed by the panelists.

Dr Swapnali Hazarika, CSIR-NEIST during the panel discussion

Day - 2: August 26, 2020

Keynote Lectures

The second day of the conference commenced with two Keynote Lectures by Dr Sanjay Singh from Gennova Biopharmaceuticals Limited, Pune on "Innovations – Transforming Healthcare" and Dr Navin Khanna, an Emeritus Scientist from ICGEB, New Delhi on "Laboratory Research: So What & What Next". This session was chaired by Dr Rakesh Mishra, Director, TIGS, Bengaluru and Professor Alok Dhawan, Director, CBMR, Lucknow.

Dr Sanjay Singh spoke on the treatment modalities for Acute Lymphoblastic Leukemia (ALL) and use of Asparaginase for its treatment. He mentioned that Gennova Biopharmaceuticals Ltd. is the first Indian company that is actively working on asparaginase formulations, and ensuring its availability in the Indian market so that all patients of this particular disease can have access to affordable treatment. He also shared his experience of the mRNA platform for the COVID-19 vaccine as well as other diseases. Dr Singh highlighted the role of women scientists in his organisation and exhorted the young scientists to seriously consider working in the corporate sector.

Dr Sanjay Singh, CEO, Gennova Biopharmaceuticals Limited, Pune delivering the Keynote Lecture

Dr Navin Khanna, ICGEB delivering the Keynote Lecture

Dr Navin Khanna shared his academic journey towards developing a procedure for dengue diagnosis that has made a big impact on public health. He mentioned the opportunity for such translational research exists for every student/supervisor in academic labs and the most important question towards this transformation would be "So What & What Next" in research practice. Even academic research efforts could make Bharat a self-reliant country, he added. Emphasizing the women's power, he quoted the lines "Lord, you are greater than my father, but just equal to my mother". He talked about the genius Indian women scientists whose inventions and experiments have helped in the progress of science and technology.

Theme – 5: Women Shaping S&T Ecosystem

This session was chaired by **Dr Shailja Bhattacharya** former Chief Scientist from CSIR-CDRI and **Dr Vandita Srivastava** from QCS Herbals.

Dr Shailja Bhattacharya, CSIR-CDRI and DrVandita Srivastava, QCS Herbals chairing the session

Dr Ritu Trivedi, CSIR-CDRI delivering a Plenary Lecture

In this session, **Dr Ritu Trivedi** from CSIR-CDRI, Lucknow delivered the first plenary lecture on "Reverse Pharmacology Approach to Drug Discovery for the Aging Bones". She summarized the current and past research efforts in her lab on the discovery of osteogenic and chondrogenic agents for primary osteoporosis and osteoarthritis.

In the second plenary lecture, **Dr Binita Phartiyal** from DST-BSIP, Lucknow spoke on "Opportunities and Challenges in Polar Earth-Sciences". She dwelled on the challenges that one has to face during long expeditions required for this field which is far away from civilization. Particularly, how the experience can be for women aspirants, and she narrated some examples. She said that the trip to the poles is exciting, unique, full of surprises and seeing, breathing and living the textbooks that were once read. It also provides an opportunity to collect the baseline data for climate research and landscape evolution of the last millennia.

Dr Ritu Trivedi, CSIR-CDRI and Dr Bushra Ateeq, IIT-Kanpur panelist during the discussion

Next, a panel discussion was held in this session which was moderated by Dr Ritu Trivedi from CSIR-CDRI, Lucknow& Dr Binita Phartiyal from BSIP, Lucknow. Dr Susheela K Branham from Bio Valley Incubator & AMTZ, Visakhapatnam; Dr Puja Panwar Hazari from DRDO-INMAS, New Delhi; Dr Bushra Ateeq from Indian Institute of Technology, Kanpur and Dr Vatsala Thirumalai from National Centre for Biological Sciences, Bengaluru were present as the panel members.

It was an interactive session, where in order to improve the performance of female scientists today, the panelist discussed challenges and coping strategies. Panelists concluded that women scientists face numerous challenges that can hinder their personal and professional development. Female scientists' well-being and productivity can be improved through both intrinsic (personal) and extrinsic (institutional) factors.

Theme – 6: Science Policy, Journalism, Information & Communication

This session was chaired by Dr Prabodh Kumar Trivedi, Director, CSIR-CIMAP, Lucknow and Dr Ritu Trivedi a Principal Scientist from CSIR-CDRI, Lucknow.

Ms. Subhra Priyadarshini, Nature-India delivering a Plenary Lecture

In this session, **Ms. Subhra Priyadarshini** from Nature-India, New Delhi delivered the first plenary lecture. She talked about alternate career opportunities and pointed out that positions as a science writer or editor in scientific journals are emerging in recent years. Based on an increasing number of journals and publishing houses in STEM, this profession is becoming exciting and much more rewarding for many science graduates, she added. She also mentioned that women scientists with a flair for writing should explore the possibilities of writing content for newspapers in India and abroad as well as for blogs, book reviews and other related online platforms.

Dr C.M. Nautiyal from Indian National Science Academy, New Delhi delivered the second plenary lecture. Drawing also from his several decades' experience, Dr C.M. Nautiyal gave an illustrated overall view of the Indian sci-com scenario over time, elaborating on high and low points. Citing instances of Total Solar Eclipse etc., he showed how media can influence the thoughts and behaviour of people. He briefed on sci- com activities of INSA and citing the results of competitions organised by INSA-SERB, he highlighted the increasing dominance of women in sci-com. He also introduced the participants on the DST's AWSAR programme.

Dr C.M. Nautiyal, INSA delivering a Plenary Lecture

The panel discussion which followed was moderated by Ms. Subhra Priyadarshini from Nature-India, New Delhi and Professor Alok Dhawan from CBMR, Lucknow. Dr C.M. Nautiyal and Dr Neelima Mishra from ICMR-NIMR, New Delhi were the panel members.

Chairpersons and Panelist during the session Science Policy, Journalism, Information & Communication
L-R: Dr C.M. Nautiyal, INSA; Ms. Subhra Priyadarshini, Nature-India; Dr Prabodh K. Trivedi, CSIR-CIMAP, Dr Ritu Trivedi, CSIR-CDRI; Professor Sandeep Verma, SERB;Professor Alok Dhawan, CBMR and Dr Neelima Mishra, ICMR-NIMR

Dr Neelima Mishra from ICMR-NIMR informed that Science and Engineering Research Board (SERB) has multiple opportunities for women in science as well as for regular researchers at various levels. She informed that the fundamental tenets of the new Science, Technology, and Innovation Policy (STIP) are being decentralized, evidence-informed, bottom-up, experts-driven, and inclusive. She encouraged the researchers and educators to read the government's recent STI policy for more information about the inclusive details and available opportunities.

The panel discussion focused on the uncertainty associated with scientific information and the challenges it poses for science communication and the way forward.

Dr C.M. Nautiyal has informed the participants about the DST- AWSAR competition, which welcomes contributions from Indian citizens actively pursuing a PhD or Postdoctoral fellowship in any field of Science and Technology (S&T).

Ms. Subhra Priyadarshini suggested that one must improve his/her writing skills to become a good science communicator.

Theme – 7: Innovation in Entrepreneurship

This session of the conference was chaired by Dr Navin Khanna from ICGEB, New Delhi and Professor Alok Dhawan, CBMR, Lucknow.

Dr Rakesh Mishra, TIGS, delivering a Plenary Lecture

Three plenary lectures were organised in this session. **Dr Rakesh Mishra**, Director, TIGS, Bengaluru delivered a lecture on the genomic approach to human diseases. He talked about his study of air surveillance of SARS-CoV-2. He also added that the air surveillance technique is not just limited to coronavirus, but can also be optimized to monitor other airborne infections. He suggested strategies to control the spread of infections like wearing masks and maintaining distance etc. Dr Mishra said "we have to learn to live with the virus" urging people to follow prevention guidelines.

Er Ajay Jain, CEO, Microlit India, Lucknow delivered the second lecture. Er Jain talked about the challenges he faced in his entrepreneurial journey and what he learned from them. Commemorating the theme of the event, he said that now science is no more gender bias. He also highlighted that all the major positions in his organisation are headed by women. He discussed the opportunities for startups in India and invited the young and enthusiastic women researchers to join the corporate world.

Er Ajay Jain, Microlit India,delivering a Plenary Lecture

Dr Vandita Srivastava, QCS Herbals delivering a Plenary Lecture

Dr Vandita Srivastava from QCS Herbals was the third speaker. She delivered a lecture on the importance of bioactivities and nutraceuticals as well as the development of nutraceuticals formulations for controlling COVID-19.

Valedictory function

The two-day conference culminated in a Valedictory session on the evening of August 26, 2022.

During the welcome address of the function, Professor Alok Dhawan, Director, CBMR profusely thanked SERB for supporting the two-day event "Women Driving Science and Technology in India". He expressed his gratitude to Secretary, SERB, Professor Sandeep Verma for taking this initiative that has brought about a positive change in the way women are taking science as a career. He also thanked the speakers for their graceful presence and sharing the motivating thoughts.

Dr Neelima Mishra from ICMR-NIMR, New Delhi offered an apt conclusion to the conference with specific summing up of the theme of the conference and the acknowledgment of the efforts of team CBMR and Professor Sandeep Verma, Secretary, SERB for choosing Uttar Pradesh for conducting such an event.

Dr Navin Khanna an Emeritus Scientist from ICGEB, New Delhi said in his remarks that this event was a benchmark for any conference and appreciated the contribution of luminaries from diverse fields in science and technology.

Professor Alok Dhawan, Director, CBMR welcoming the guests during the Valedictory Function

Professor Sandeep Verma, Secretary, SERB and Chief Guest of the function congratulated the organizing committee for the successful organization of the two-day event. He emphasized the significance of empowering the women researchers in our S&T landscape. He briefed the gathering about the SERB-POWER (Promoting Opportunities for Women in Exploratory Research) Scheme, which has two verticals of POWER-Fellowship and POWER-Research grants. This scheme is exclusively designed for women scientists to mitigate gender disparity in science and engineering research in various science and technology (S&T) programmes.

Chief Guest, Professor Sandeep Verma, Secretary, SERB delivering Valedictory Address

He said that this initiative of SERB will serve as a benchmark of recognition in the national scenario and will empower women scientists and cultivate a women-friendly culture and ensure more women in leadership positions in decision-making bodies. Professor Verma informed that SERB has added two new verticals in this exclusive program for female researchers: POWER-translation grant to enhance research readiness levels and POWER-mobility grant to work in international laboratories. At last, he suggested that,it would be good to organise another UP-centric event in which the women young scientist and PhD students would present their scientific contributions in the form of lectures/ poster presentations. This will further build confidence in them as well as enable them to showcase cutting-edge research being done at their respective scientific institutions in Uttar Pradesh.

Professor Neeraj Sinha, Dean, CBMR proposed Vote of Thanks on behalf of the Organising Committee and hoped that CBMR should be able to organise more such Conferences in future.

The two-day national event on "*Women Driving Science and Technology in India"* organised by the Centre of BioMedical Research (CBMR), Lucknow, had a wrap up with following recommendations from the discussions held during the event:

Professor Alok Dhawan, Director, CBMR felicitating the Chief Guest,
Professor Sandeep Verma, Secretary, SERB during the Valedictory Function

RECOMMENDATIONS:

1 To encourage more and more women into S&T, such programmes should be conducted at regular intervals and across the country especially where the number of women in S&T is less.

2. An all women symposium on a selected field of S&T should be organised for showcasing of research as well as better networking.

3. Creating more opportunities for mentoring and collaboration in the aligned research areas and industry-oriented work. Mobility grants should be given to women to travel within the country to undertake high-end research for a period of 3-6 months during their PhD or early career.

4. Women centric bilateral travel grants should also be initiated for networking and to enhance diversity in research institutes. This will help young women scientists to visit labs in their area of research abroad and get exposure at an early stage of their career.

5. All women scientists' workshops on specific techniques should be encouraged to build confidence among the PhD students and also build capacity.

6. Workplaces should be made more women friendly such as a mandatory creche, transport support etc.

7. Organisation of STEM hackathons to promote innovation, translational research, new knowledge generation and evidence-based research for women researchers.

National Sudden Cardiac Arrest

Awareness Week

September 24, 2022

National Sudden Cardiac Arrest Awareness Week on September 24, 2022 was organised at CBMR to raise awareness about sudden cardiac arrest (SCA). On this occasion, Professor Aditya Kapoor, Head, Department of Cardiology, SGPGIMS, Lucknow educated the CBMR staff, faculty and students about the risk factors for SCA and how to respond in case of an emergency.

Gandhi Jayanti

October 02, 2022

To commemorate the 153rd birthday of Mahatma Gandhi, CBMR conducted a Special Assembly on Gandhi Jayanti on October 2, 2022. On this occasion, the Director, staff, faculty and students of CBMR paid their heartfelt tributes to the Father of the Nation.

1st Academic Council Meeting

October 11, 2022

The Academic Council is the principal academic body of the Centre. The 1st Meeting of the Academic Council was held on October 11, 2022 under the Chairmanship of the Director, CBMR, Professor Alok Dhawan.

Professor Neeraj Sinha, Dean, CBMR; Dr Saumen Hajra, Professor, CBMR, Professor Shubha Phadke, HOD, Department of Genetics, SGPGIMS; Professor Surya Kant, HOD, Department of Respiratory Medicine, KGMU, Lucknow; Professor Abbas Ali Mahdi, HOD, Department of Biochemistry, KGMU, Lucknow; Dr Uttam Kumar, Additional Professor, CBMR; Dr. Syed Masood Husain, Associate Professor, CBMR; Dr Biswanath Maity, Associate Professor, CBMR participated in the meeting and gave their valuable suggestion for running the academic programme for CBMR.

9th Scientific Advisory Committee Meeting

October 14, -Oct-2022

The 9th Scientific Advisory Committee Meeting of CBMR was held on October 14, 2022 under the Chairmanship of Dr C.M. Gupta, Distinguished Professor, Institute of Bioinformatics and Applied Biotechnology, Bengaluru.

Following member attended the meeting Dr Rakesh Mishra, Director, TIGS, Bengaluru; Dr Rohit Srivastava, Professor, IIT-B, Mumbai; Professor R.V. Hosur, Former Senior Professor, TIFR, Mumbai; Dr G. Narahari Sastry, Director, CSIR-NEIST, Jorhat; Professor N.R. Jagannathan, Professor of Eminence Radiology, Chettinad Hospital and Research Institute, Chennai; and Dr C.V. Ramana, Principal Scientist, CSIR - NCL, Pune and Professor Alok Dhawan, Director, CBMR. The faculty made presentations regarding the progress of their research work and the SAC members gave suggestions on how to enhance translational outcomes.

L-R: Dr Rakesh Mishra, Dr Rohit Srivastava, Dr C.M. Gupta, Professor Alok Dhawan, Professor R.V. Hosur, Dr G. Narahari Sastry, Professor N.R. Jagannathan

Inauguration of 3D Bioprinting Lab

October 14, 2023

A 3D Bioprinting Lab was inaugurated on October 14, 2023 at CBMR by Dr C.M. Gupta, Chairman, SAC and Distinguished Professor, Institute of Bioinformatics and Applied Biotechnology, Bengaluru. The lab will be utilized for 3D bioprinting, a rapidly advancing technology for transitional biomedical research. By combining living cells and biomaterials, complex 3D structures will be created that may be transplanted into patients. These structures can also be utilized to create disease models, allowing for greater insights into disease progression and potential treatment options.

Training Workshop on

Recent advances in 3D bioprinting of living tissues and its emerging applications in biomedical research

November 07, 2022

A hands-on training workshop on "Recent advances in 3D bioprinting of living tissues and its emerging applications in biomedical research" was organised by the Department of Biomedical Engineering and Devices of CBMR in association with M/s Biotron Healthcare on November 7, 2022. The workshop was attended PhD students, academic research scholars and faculty members. The demonstration on 3D bioprinting was conducted by the application engineer of M/s Biotron Healthcare.

Professor P.K. Seth, Former CEO, Biotech Park was the Chief Guest and inaugurated the workshop. Professor Alok Dhawan, Director, CBMR welcomed the participants. The inaugural session included a brief keynote lecture by Professor P.K. Seth on various applications of 3D bioprinting. Professor Neeraj Sinha introduced various biomedical research facilities and activities of CBMR.

The scientific session included one keynote lecture by Dr. Krishna Mohan Poluri, Associate Professor, IIT Roorkee, and four invited lectures, including one from the National Institute for Materials Science (NIMS), Tsukuba, Japan. The speakers highlighted the importance of 3D bioprinting in fields such as the development of scaffolds for tissue engineering, 3D cell culture models (including those of certain diseases) for evaluating therapeutic efficacy and safety of promising candidate drugs or drug formulations, and more.

Overall, the workshop conducted at CBMR helped create awareness among young researchers about 3D bioprinting and its emerging applications, especially in the medical and pharmaceutical industries.

One-day Conference on
Emerging Healthcare Technologies

December 17, 2022

Center for BioMedical Research (CBMR) and Innovation Hub, AKTU in association with KGMU, StartinUP and Industry Academia Knowledge Alliance (IAKA) have jointly organized a one-day conference on “Emerging Healthcare Technologies” on December 17, 2022. The conference was attended by almost 500 medical doctors, diagnostic companies, med-tech startups, IT professionals, and students from the biomedical sector.

The conference aimed to emphasize the importance of technology in the healthcare sector, including access to medical information and data, telemedicine / tele-health, and electronic health records. These technologies assist physicians, nurses, and other care givers in treating patients, leading to improved outcomes, health system savings, and economic growth.

विज्ञान संगम

Lecture Series

Lecture –1

April 1, 2022

Professor Akhila Kumar Sahoo

University of Hyderabad

Title: Cationic-Palladium Catalyzed Regio- and Stereoselective Dicarbofunctionalization of Unsymmetrical Alkynes

Lecture – 2

September 30, 2022

Professor Pankaj Seth

Scientist VII
Molecular and Cellular Neuroscience, Neurovirology
Section National Brain Research Centre
Manesar, Haryana

Title: Human fetal brain derived neural stem cell model and its potential for understanding healthy and diseased brain

Lecture – 3

December 13, 2022

Professor Subhash C. Pandey

Director, Alcohol Research Center
Department of Psychiatry, University of Illinois at Chicago and
Senior Research Career Scientist
Jesse Brown VA Medical Center, Chicago, USA

Title: Epigenetic Regulation in Alcohol Use Disorder: Phenotypes, Mechanisms and Treatment

Interactive Meet

April 20, 2022

CBMR organised an interactive meet on April 20, 2022 with bright, innovative and energetic CSIR-UGC NET JRF qualified students of University of Lucknow.

During the meeting, CBMR faculty shared valuable insights into their cutting-edge research endeavors. The aim of the meeting was to foster knowledge exchange and encourage the students to engage in innovative research practices. The attendees were highly engaged and enthusiastic, and the event served as a great opportunity for CBMR to showcase their work to a talented group of young scholars.

Distinguished Visitor

April 04, 2022

Professor N. R. Jagannathan

Adjunct Professor
Department of Electrical Engineering IIT
Madras, Chennai

Professor N. R. Jagannathan visited CBMR on April 04, 2022 to review and evaluate the ongoing projects on Nuclear Magnetic Resonance (NMR) and Magnetic Resonance Imaging (MRI). The faculty members of Department of Advanced Spectroscopy and Imaging reaped multiple benefits from his visit.

Faculty / Students Visits to CBMR

In accordance with CBMR's scientific social responsibility, many undergraduate and postgraduate students from various institutions visited the Centre during the year. The purpose of these visits was to provide the students with firsthand knowledge and experience of the ongoing research activities at the Center. This initiative allowed the students to gain valuable insights into the scientific processes and methodologies employed by CBMR, thus enabling them to enhance their knowledge and skills in their respective fields of study.

Visit – 1

June 20, 2022

University of Lucknow, Lucknow
Department – B.Pharma

Visit – 2

June 29, 2022

University of Lucknow, Lucknow

PhD/Postgraduate Students of Institute of Advanced Molecular Genetics & Infectious Diseases (IAMGID)

Visit – 3

July 30, 2022

Chhatrapati Sahu Ji Maharaj University (CSJMU)
(Formerly Kanpur University, Kanpur)
M.Sc. Students from Department of Life Sciences & Biotechnology

Visit – 4

August 08, 2022

Amity University, Lucknow

M. Pharm (Pharmaceutics & Pharmacology) and PhD students of Amity Institute of Pharmacy

Visit – 5

August 16, 2022

Shri Ramswaroop Memorial University (SRMU), Lucknow
B.Tech students of Center of Innovation, Incubation, and Entrepreneurship (CIIE)

Visit – 6

October 18, 2022

Amity University, Lucknow

M Tech/B Tech and PhD students of Amity Institute of Biotechnology

Memorandum of Understanding (MoU)

CBMR - AIIMS, Jodhpur

A memorandum of understanding was signed between CBMR and AIIMS, Jodhpur on February 4, 2022 to undertake joint clinical and translational research.

CBMR & University of Lucknow

A memorandum of understanding was signed between CBMR and University of Lucknow on February 21, 2022 to allow students & young faculty to do collaborative research using state of the art facilities and create vibrant research eco-system.

CBMR & DBT-THSTI

A memorandum of understanding was signed between Centre of BioMedical Research (CBMR), Lucknow with DBT-Translational Health Science and Technology Institute (THISTI), Faridabad on June 08, 2022 for undertaking joint translational research.

CBMR & CSMU Kanpur

A memorandum of understanding was signed between Centre of BioMedical Research (CBMR), Lucknow with Chhatrapati Shahu Ji Maharaj University, Kanpur on July 6, 2022 to allow students & young faculty to do collaborative research using state-of-the-art facilities and create a vibrant research eco-system.

CBMR & KGMU, Lucknow

A Memorandum of Understanding was signed between the CBMR, Lucknow and King George's Medical University (KGMU), Lucknow on July 16, 2022 for research in various areas. It will leverage expertise available at KGMU in both basic and clinical sciences as well as interdisciplinary sciences at CBMR for better patient care.

CBMR & IIT Kanpur

A memorandum of understanding was signed between CBMR and Indian Institute Technology-Kanpur on July 6, 2022 for translational research especially in the area of AI in healthcare, biomedical devices and drug discovery.

CBMR & IIT, Bombay

A Memorandum of Understanding was signed between the CBMR, Lucknow and IIT Bombay on October 14, 2022 for translational research especially in the area biomedical devices.

Governing Council/General Body

Chairman

Shri Durga Shankar Mishra
Chief Secretary
Government of Uttar Pradesh

Vice Chairman

Dr Sanjeev Misra
Former Director, AIIMS – Jodhpur
and Vice Chancellor
Atal Bihari Vajpayee Medical
University (ABVMU), Lucknow

Members

Dr C.M. Gupta
Chairman, Scientific Advisory
Committee (SAC) and
Distinguished Professor, IBAB
Bengaluru

Professor Jayesh Bellare
Institute Chair Professor
Indian Institute of Technology-Bombay

Dr. Sanjay Singh,
Chief Executive Officer
Gennova Biopharmaceuticals Limited
Pune

Shri Anupam Jalote
Former Chief Executive Officer
iCreate, Ahmedabad

Shri Alok Kumar
Principal Secretary
Medical Education Department
Government of Uttar Pradesh

Shri Prashant Trivedi
Additional Chief Secretary
Finance Department
Government of Uttar Pradesh

Dr Rajesh S Gokhale
Secretary
Department of Biotechnology
New Delhi

Dr. Srivari Chandrasekhar
Secretary
Department of Science & Technology
New Delhi

Dr N Kalaiselvi
Director General,
Council of Scientific & Industrial
Research, New Delhi

Dr Rajiv Bahl
Director General
Indian Council of Medical Research
New Delhi

Professor Alok Dhawan
Director
Centre of BioMedical Research
Lucknow

Professor R.K. Dhiman
Director
Sanjay Gandhi Postgraduate Institute
of Medical Sciences, Lucknow

Administrative Officer of CBMR shall be the Non-Member Secretary of the Council

Scientific Advisory Committee

Chairman

Dr. C.M. Gupta
Distinguished Professor
Institute of Bioinformatics and Applied Biotechnology
Bengaluru

Members

Dr N.R. Jagannathan
Adjunct Professor, Department of Electrical Engineering
IIT - Madras, Chennai and
Advisor, Chettinad Hospital & Research Institute Kelambakkam and
Former Professor & Head, Department of NMR & MRI Facility
AIIMS, New Delhi

Dr D. Srinivasa Reddy
Director
CSIR-IICT Indian Institute of Chemical Technology
Hyderabad and Former Director
CSIR – IIIM, Jammu

Dr Rakesh K. Mishra
Director
Tata Institute for Genetics and Society
Bengaluru and
Former Director
CSIR-CCMB
Hyderabad

Dr Radha Rangarajan
Director
CSIR-Central Drug Research Institute
Lucknow

Dr Rohit Srivastava
Himanshu Patel Chair Professor
Department of Biosciences and Bioengineering
Indian Institute of Technology - Bombay
Mumbai

Member Secretary

Professor Alok Dhawan
Director
Centre of BioMedical Research
Lucknow

Academic Council

Chairman

Professor Alok Dhawan
Director
Centre of BioMedical Research
Lucknow

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Lucknow

Dr Saumen Hajra
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Professor & Head
Department of Medical Genetics
Sanjay Gandhi Postgraduate Institute of Medical Sciences
Lucknow

Dr Surya Kant
Professor & Head
Department of Respiratory Medicine
King George's Medical University
Lucknow

Dr Abbas Ali Mahdi
Professor & Head
Deparment of Biochemistry
King George's Medical University
Lucknow

Dr Sharad Sharma
Chief Scientist
Department of Molecular & Structural Biology
CSIR-Central Drug Research Institute
Lucknow

Dr Uttam Kumar
Additional Professor
Centre of BioMedical Research
Lucknow

Dr Syed Masood Husain
Associate Professor
Centre of BioMedical Research
Lucknow

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CBMR research was generously supported by the U.P. Government

Funding

	Rs. in Lakhs
UP Government	1,716.96
Extramural Funding	215.10
Total	1,932.06

Extramural Projects funding Agencies

ICMR
INDIAN COUNCIL OF MEDICAL RESEARCH

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सत्यमेव जयते
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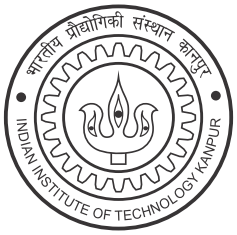



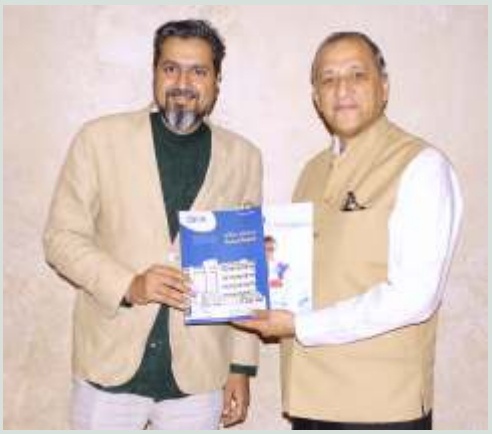






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CBMR

जैव चिकित्सा अनुसंधान केन्द्र

Centre of BioMedical Research

उत्तर प्रदेश सरकार का स्वायत्तशासी केन्द्र

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